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Robert W. Lyczkowski

The History of Multiphase Science and Computational Fluid Dynamics

A Personal Memoir

Springer

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This book is dedicated to Prof. Dimitri Gidaspow, Distinguished University Professor at the Illinois Institute of Technology, Department of Chemical and Biological Engineering.

I have had the unique opportunity and pleasure to have been a student and then collaborator with Dimitri for over 40 years! Our first publication together was in 1967 resulting from my MS thesis under him. Our most recent publication was in 2009 with one of his last Ph.D. students. I think that this is probably some sort of record at IIT. I was incredibly lucky to have participated at the birth of the new science of multiphase flow started by his first student, Dr. Charles W. Solbrig and propagated by Dimitri. I have been co-advisor and assisted a good number of Dimitri's Ph.D. students. As I said at his retirement party, I have followed in his footsteps, figuratively and actually over the years—San Francisco, Atlantic City, Denver, Idaho Falls, Livermore, Washington DC, Henniker, Banff, Miami Beach... When we gave a multiphase course in Melbourne, Australia I drove him to the beach everyday *to swim which he does everyday to keep in shape. Congratulations Dimitri on your retirement from IIT but not from research. Your friend and colleague, Bob Lyczkowski.*

It is also dedicated to Charles W. Solbrig, Dimitri's first student. It was he who was the first to develop the equations and to initiate the computer program to solve them which were based on the two-phase, two-fluid or seriated continuum approach.

Foreword

It is a great honor for me to provide the Foreword for a book by the distinguished engineering scholar Bob Lyczkowski, who I have known for many years through his association with Argonne National Laboratory. In his work at Argonne and elsewhere, Bob has contributed immeasurably to the application of multiphase flow analysis in industrial processes.

When the US Atomic Energy Commission (later integrated into the US Department of Energy) was formed in the early 1950s with a mission to develop nuclear reactors for civilian applications, most of the fundamental engineering research conducted at National Laboratories in support of the civilian nuclear reactor programs focused on materials and on heat transfer. It was recognized that there were no fundamental approaches to multiphase flow and heat transfer, and the US Government organized major programs in fundamental research of multiphase flow and heat transfer at Los Alamos NM, Idaho Falls, Sandia Albuquerque, and elsewhere.

Some people who are familiar with the mechanics of a single fluid phase and gas dynamics are unaware of the striking and profound differences exhibited by multiphase flows, even in dilute two-phase mixtures. Many flow regimes appear in two-phase flows that are unknown in single-phase flows, and a considerable amount of heat transfer phenomena are exhibited by two (or three)-phase flow regimes that are not exhibited by single-phase fluid flows.

It is a profound challenge to provide a mathematical description of multiphase flow and heat transfer, and to provide fundamental understanding of observed multiphase flow phenomena—either from a continuum or microscopic approach. Extraordinary advances in these areas have come from such renowned figures as Dimitri Gidaspow, Milorad Dudukovic—and Bob Lyczkowski himself. Their work has provided the backbone of numerous commercial and proprietary multiphase software analysis packages, which have made multiphase flow analyses accessible to the non-expert.

In this book, Bob examines the development of multiphase flow analysis methods and software approaches and also discusses some political and societal influences on the development of these. In this manner, Bob's book becomes a history of this field of engineering. Bob also provides the only history I am aware of the Multiphase Fluid Dynamics Research Consortium supported by the US Department of Energy nearly twenty years ago, involving numerous National Laboratories, Universities, and private businesses. For Bob's history and discussion, I am grateful.

I hope many readers find this book enlightening and entertaining, and I hope that all students beginning Master's or Ph.D. level studies of multiphase flow will make this the very first book they read on the subject.

May 2017

Brian Gregory Valentine
US Department of Energy, Washington, DC, USA

Preface

> Those who cannot learn from history are doomed to repeat it.
>
> George Santayana
>
> Insanity: Doing the same thing over and over again and expecting different results.
>
> Albert Einstein

The idea for this book on *The History of Multiphase Science and Computational Fluid Dynamics* (CFD) can be traced to a presentation I made upon my receiving the 2008 Ernst W. Thiele Award from the Chicago Section of the American Institute of Chemical Engineers (AIChE) on September 22. I prefaced the presentation ceremony with a short speech beginning with the question "Where did these equations come from?" The idea for writing a book to answer this question strengthened as I organized two sessions at the 2009 AIChE Annual Meeting in Nashville, with help of Madhava Syamlal from the National Energy Technology Center (NETL), to honor our teacher from the Illinois Institute of Technology (IIT), Prof. Dimitri Gidaspow with a Festschrift to honor his 75th birthday. I should mention that Prof. Gidaspow (whom I will frequently refer to simply as Dimitri in context) was a previous recipient of the Ernst W. Thiele Award and was the one who nominated me. Upon the suggestion of Madhava Syamlal (called Syam by his colleagues) and with the generous assistance of Prof. Sankaran Sundaresan from Princeton University, we convinced Donald R. Paul, then the Editor of I&EC Research, to publish a special Festschrift for Prof. Gidaspow. Invitations were sent out to over 50 potential contributors, and a total of 31 papers were published with a preface by the three of us.

The story of multiphase science and computational fluid dynamics (CFD) has never been documented heretofore. This may surprise some readers, but the motivation for modeling transient two-phase flow started with nuclear reactor water safety concerns, the hypothetical loss-of-coolant accident (LOCA), and the emergency core cooling system (ECCS) issue. It is a new and by now a rather robust science and one which must be told how it came to be before the founders and key contributors pass on. Unfortunately, this has already begun to occur. At least three have done so, and a couple more nearly did.

I was helped in this endeavor with the cooperation of Dimitri Gidaspow, Charles W. Solbrig, Lawrence J. Ybarrondo, Victor H. Ransom, John Ramshaw, and E. Daniel Hughes, all major players in the story, with whom I have had considerable correspondence through emails and telephone and personal conversations over the past several years. If anyone of an amazing chain of incidents, and coincidences had never happened, multiphase science and CFD would never have evolved and the story this book tells would never have materialized. It is almost as though the unfolding of these events had been predestined as described in Part I. I will do my best to convince the reader this is so. The remainder of the book recounts incidents which I call the politics of science and the failure to establish a truly national initiative for multiphase computational fluid dynamics. The book concludes with some of the lessons learned from writing this book and how multiphase science and CFD might or should be applied in the future.

Darien, USA Robert W. Lyczkowski

Contents

About the Author

Robert W. Lyczkowski received his BChE in from Cleveland State University, Fenn School of Engineering and MS in Gas Engineering and Ph.D. in Gas Technology from Illinois Institute of Technology. He worked for Lawrence Livermore National Laboratory, Idaho National Engineering Laboratory, Energy Incorporated, Goodyear Atomic Corp., Hooker Chemical Corp., and as a faculty member at Illinois Institute of Technology. He has been involved for over forty years in chemical and nuclear engineering applications of his multiphase theory and computational fluid dynamics expertise, especially in the areas of heat transfer and energy conversion to develop models that are now used by industry worldwide to design various two-phase flow equipments. He is a Fellow of the American Institute of Chemical Engineers and a recipient of the prestigious Ernst W. Thiele Award.

Most of Dr. Lyczkowski's career was spent as a Chemical Engineer in the Energy Systems Division at Argonne National Laboratory. He was involved with computer modeling of fluidized beds and dense slurries. His expertise is in the areas of multiphase flow and heat transfer, erosion, light water and liquid metal nuclear reactors, in-situ processing of fuels, and concentrated suspensions. He applied multiphase dense slurry modeling to the development of a unique non-Newtonian power-law model for multiphase hemodynamics. This established a completely new paradigm for analyzing the migration of blood-borne particulates. This model was used to develop a mechanistic monolayer population balance cell-adhesion model to aid in determining the threshold conditions of atherosclerosis initiation and progression. He was involved with modeling a novel multiphase concept involving chemical water splitting using high-temperature steam bubbling into a bath of molten calcium bromide as the first step in the calcium–bromine (Ca–Br) cycle.

He is the author of over 150 technical publications (over 50 refereed journal articles and book contributions and over 100 conference papers), over 50 reports, and holds two US patents. He contributed significantly to the development of the RETRAN and COMMIX computer programs. He has recently completed a book titled "The History of Multiphase Science and Computational Fluid Dynamics a Personal Memoir."

Chapter 1
Introduction

This book presents my personal recollections tracing the most signal events in the history of the initiation, development, and propagation phases of multiphase science and computational fluid dynamics (CFD) which initiated in 1970 in a state far away. There are overlaps in the transitions from one phase to another. I define the initiation phase as beginning with Charles W. (Charlie) Solbrig and Lawrence (Larry) J. Ybarrondo circa 1970 and ending in 1975 with the dissolution of the original SLOOP (Seriated LOOP) code group at Aerojet Nuclear Company (ANC). This is described in PART 2, which constitutes the central core of this book's story.

The development phase extends from 1975 to roughly 1992–1993. The fragments from the SLOOP code development were taken up by Victor (Vic) H. Ransom who, together with Richard (Dick) J. Wagner and John A. Trapp, initiated and developed the RELAP5 code [1]. It should be mentioned at this point to the reader unfamiliar with CFD that the word "code" is used in this book interchangeably with the term "computer program." RELAP5 is described in PART 3, which also chronicles the rise of other multiphase CFD codes on the part of the US Nuclear Regulatory Commission (NRC) to better analyze light water and sodium-cooled fast reactors and the US Department of Energy (DOE) to grapple with the energy crises caused by the Arab oil embargo in the 1970s. Subsequently, the development history of multiphase science splits into two distinct and independent paths: (1) a series of water-cooled nuclear reactor safety codes, including RELAP5 developed at the Idaho National Laboratory (INL) and water- and sodium-cooled nuclear reactor codes developed at the Los Alamos National Laboratory (LANL) and (2) codes developed by Dimitri Gidaspow at IIT to model fluidization. Eventually commercial codes would contain the essence of multiphase science initiated by him and his students.

The propagation phase extends from 1994 to the present starting with the publication of Dimitri Gidaspow's first book [2]. PART 4 describes the efforts to establish a national program for multiphase flow. These efforts eventually wound up as a de facto program at NETL. PART 5 describes the influence of Dimitri's book on the international stage. While not claiming to be definitive nor complete, this

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book has as its primary objective the documentation of some of its most significant milestones and events. The history of multiphase science and CFD is intimately and inextricably connected with a significant portion of the career of Dimitri Gidaspow, now Distinguished University Professor Emeritus at the Illinois Institute of Technology (IIT). He was honored with a Festschrift for his 75th birthday at the 2009 AIChE Annual Meeting in Nashville, TN, November 8–13, and subsequently with a special issue of I&EC Research [3] for which I contributed the article "The History of Multiphase Computational Fluid Dynamics" [4]. This I&EC special issue contains invited contributions from colleagues, former students, and experts in multiphase science, especially in the fields of fluidization and solids transport. Madhava Syamlal and Professor Sankaran Sundaresan assisted me in preparing an introductory article to the I&EC Dimitri Gidaspow Festschrift [5]. A very brief account from a different perspective was presented at "A Festschrift to Honor Professor Dimitri Gidaspow on His 65th Birthday" which I organized at the 33rd National Heat Transfer Conference, August 15–17, 1999, in Albuquerque, NM [6]. Special emphasis is placed upon the initiation phase since it has not been formally documented previously, to my knowledge. The most recent Festschrift for Dimitri was held at the AICHE Annual Meeting in Atlanta, November 18–21, 2014. The two sessions were divided into (1) presentations by his former students and colleagues invited by me and (2) presentations by a roster of contributors from universities and research establishments invited by Madhava Syamlal. He and I alternated as session chairs. To give an idea of the international influence of Dimitri, presenters traveled from China, France, and England.

When I wrote my I&EC article for the Dimitri Gidaspow Festschrift [4], the description of the initiation phase was limited by time and length limitations which I will make up for in this book. I was unaware of the interaction of Charlie Solbrig with LANL's Group T-3 as the SLOOP code program was being initiated. I was also unaware of the back story of the sustained effort on the part of Long Sun Tong (frequently shortened to just L.S. Tong), Assistant Director for Water Reactor Safety Research at the NRC, to deliberately destroy this program in the 1970s. I was totally unaware of this fact when I was working in the SLOOP code group from 1972 to 1975. Now this aspect of the story can be told.

A remarkable group of individuals were assembled by Larry Ybarrondo and Charlie Solbrig in Idaho at what was then the National Reactor Testing Station (NRTS) (now the Idaho National Laboratory) to develop what came to be called the SLOOP code. It was intended to replace the RELAP4 code, to be discussed in Chap. 4, used to perform safety studies for and to license nuclear reactors.

This book rights the slights of Stan Fabic's brief survey of best-estimate codes funded by the NRC [7] and in the book describing the history of the Idaho National Engineering and Environmental Laboratory (INEEL) from 1949 to 1999 [8]. RELAP5, which will be discussed in Chap. 10, is mentioned only once on page 6-201 in Fabics's survey. There is no mention at all of the SLOOP code effort. There are only two short paragraphs on pages 226 and 230 of the INEEL history describing the development of the RELAP series of nuclear reactor safety codes including RELAP5. There is a terse description on page 225 of the role such codes (unnamed) played in the analysis of the accident at the Three Mile Island nuclear power plant on March 29, 1979.

Carl Hocevar, who was a member of the SLOOP code development effort, mentioned in his 1975 critique of computer safety predictions methods that ANC "…has been developing an unequal velocity-unequal temperature model for several years" [9]. He stated in the addendum that "The new thermal-hydraulic computer code development program at Aerojet Nuclear Company…has now been terminated." This program was not even mentioned in the book on the history of the INEEL [8]. No names are associated with these nuclear reactor codes. One goal of this book is to put a human face on the development of them and their role in predicting nuclear safety validation experiments.

Coming back to the history of multiphase science, I should mention the article by Francis H. Harlow, who is universally recognized as the pioneer of CFD [10]. He describes Group T-3's experience in formulating CFD algorithms to solve the Navier–Stokes equations, turbulence, and what he refers to as multifield equations. There is no mention in this article of interaction with the Idaho group which worked on the SLOOP code nor in his most recent book of memoirs [11]. In Sect. 7, Multifield flows (1971) [10], he concedes that these equations are mathematically ill-posed giving no reference to our seminal paper [12] on the subject described in some detail in Chap. 6, nor to any other research into this subject since 1978. I actually called him on June 8, 2016, to discuss these and other issues upon which I will elaborate in Chap. 7. I might have been one of the last, if not the last, to talk with him since he died on July 1, 2016!

Even though my SLOOP code tenure lasted a little over three years from March 1972 to July 1975, the experience in hindsight was exhilarating and has made a lifetime impact on me. I became a de facto "expert" in multiphase flow modeling. My mind was expanded in a way that the emotional trip through the hoops of obtaining my Ph.D. paled by comparison.

1.1 An Apologia

I want to make it perfectly clear that this book is a personal memoir and that it covers a significant amount of time—almost six decades. In that time, the names of US national laboratories changed, some several times. Government organizations also change their names, for example the US Atomic Energy Commission (AEC) became the Energy Research and Development Administration (ERDA) and finally the US Department of Energy (DOE). When I first refer to them in a particular time frame, I use their original name and frequently state their present name. When I go back and forth in time, I cannot possibly keep track of their names and therefore mix the names. I also shorten their names. Such an example is Los Alamos National Laboratory (LANL) which became Los Alamos Scientific Laboratory (LASL). Sometimes I will just use LASL and sometimes I will just use Los Alamos. As far as the major persons in this book, there are Dimitri Gidaspow, Charlie Solbrig, Dan

Hughes, Vic Ransom, Larry Ybarrondo, etc. I will frequently use their first names in referring to them. It will be clear that there is only one Dimitri, one Charlie, one Vic, one Larry, etc. For this, I apologize and I hope the reader will tolerate this informality.

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Part I
Predestination

Wherein is told of the circumstances and fate which propelled me to meet up with Charlie Solbrig and Prof. Dimitri Gidaspow.

Chapter 2
Cleveland State University, Cleveland 1959–1964

In my paper "The history of Multiphase Computational Fluid Dynamics" [1], I began the story as starting in Chicago. Upon reflection, since writing this paper, I realized that the story actually begins earlier. I decided to attend Fenn College in Cleveland upon graduating from high school in Dunkirk, New York, in 1959. It is necessary to begin the story in Cleveland because it was there that the chain of events began which I now refer to as predestination.

I graduated as salutatorian of my class with a female beating me out by several hundredths of a grade point average. I took science and mathematics electives including physics, chemistry, biology, and the refreshing course, solid geometry. I liked solid geometry because it expanded my mind from the obviously limited (or incomplete) schooling involving Euclidean geometry. Instead of triangles having angles summing to 180°, on a sphere they summed to *greater* than 180°. Parallel lines met and did not extend to infinity. I received a New York State Regents diploma with honors in science and mathematics.

My parents were not wealthy. I was the eldest of four children with three sisters coming after myself. My father worked mostly at the Dunkirk plant of the Allegheny Ludlum Steel Corporation which manufactured specialty stainless steels in the form of rods, wire, and sheets. In the late 1950s, there was at least one other location for the Allegheny Ludlum Steel Corporation in Watervliet, New York. Sometimes when layoffs occurred and some production would be transferred to Watervliet, he would work at the Dunkirk Radiator factory or at the ALCO Products, Inc. These Dunkirk industries are either shuttered and long gone or repurposed in the rust belt constituting Western New York. The movement of steel manufacturing subsequently essentially exiting the USA eventually doomed these industries.

My father attended a local technical high school where he must have acquired the skills he would use in his future employment. My mother never graduated from high school and never really worked except during the Great Depression since her mother died when she was a youngster. She had three sisters and two brothers. To make ends meet, she and her sisters worked at the local Van Raalte garment factory which she always referred to as "the silk-mill" (long shuttered). Her brothers went

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into the army. Their father worked at the American Locomotive Company often shortened to ALCO. Apparently, it closed and was torn down around World War II and eventually morphed into ALCO Products, Inc. My parents would moonlight at a local nightclub to make ends meet. In addition, my father would moonlight as grounds keeper and maintenance man for the St. Hedwig's Catholic Church, a couple of blocks from our home. I would sometimes accompany him as an unpaid assistant. The history of my father's parents is much murkier than my mother's. It is similarly tragic in that his mother married twice with both husbands dying relatively young before I was born. She had three children by her first marriage and three more by her second husband. So, I had a lot of uncles and aunts!

But enough of this part of the distant past—on to continue my story. As I already mentioned, upon graduating from Dunkirk High School I was determined to go to college. I should put into perspective that my desire was to become an engineer. This was because of the greatly increased interest in science and technology sparked by the Soviet Union successfully launching Sputnik 1, the world's first artificial satellite on October 4, 1957. I was a junior in high school, and the excitement over Sputnik 1 was my *raison d'etat* for going to college and becoming an engineer. I applied to a good number of colleges a reasonable distance from Dunkirk in Western New York, Pennsylvania, and Northern Ohio having engineering schools and to Rensselaer Polytechnic Institute (RPI) which had a prestigious engineering school. I subjected my parents to filling out endless forms in an attempt to obtain some sort of financial assistance since they had accumulated nowhere enough savings to pay for my college tuition and dormitory housing expenses. I took the New York State Regents Scholarship examination in my senior year for which the scholarship would have been applicable only for the New York State colleges I had applied to, including RPI. Unfortunately, I was not on the top list of recipients of a New York State Regents Scholarship which was quite disappointing to me and my parents. Several of the senior year students did receive one. Financial aid was not materializing for me from the colleges I had applied to maybe because of the large crush of students entering colleges due to the effect of Sputnik 1.

What follows now constitutes the first on a chain of events in what I refer to as predestination. I ultimately decided to attend Fenn College in Cleveland, Ohio, where I applied and had been accepted. The college had a Cooperative Training Program (known as co-op), later called the Cooperative Education Program, wherein students would alternate between the classroom and practical work experience in their major field. I figured that if I didn't get any financial assistance, I could struggle through the freshman year which had three quarters (Fenn was on the quarter not the semester system) with help from my parents to pay for tuition, books, dormitory expenses, and meals. Thereafter, I figured that I could then earn enough money to cover these expenses doing my co-op. Nonetheless, I still applied for financial aid.

In January 1959, I traveled by train to Cleveland to take scholarship examinations for financial aid at Fenn College. Travel to Cleveland was easy in the 1950s and 1960s since there was a train station in Dunkirk with a direct connection to

Cleveland. This would be my first travel away from home, and I went alone. I was interviewed by Dr. V. Richard Gulbenkian, Director of Admissions and Records. I carried with me the paperback I started to read on the train by F. Scott Fitzgerald titled "Tender Is the Night." When we met, Dr. Gulbenkian noticed the book and was curious as to why I was reading this particular book. I don't remember my response, but I think he was impressed that a kid just 17 years old would be reading such exotic material. I returned to Dunkirk by train the same day and awaited the results of the tests and interview. That spring, lo and behold, I received financial assistance for the freshman year, September 1959 to June 1960. The total amount of the award was $1,000 of which $750 was a scholarship and $250 was in the form of a low-interest federal loan for which my father had to cosign a promissory note. The loan would have to be paid back starting 1 year after graduation. At which time the interest on the loan at 3% would start. For the summer quarter, 1963, I received further financial assistance in the amount of $500, $375 of which was a federal loan. The conditions for the loan were the same. The award portion was provided by the Fenn College Alumni Association.

This government-backed student loan was made available under the National Defense Education Act. These loans were only available to select categories of students such as those studying for an engineering degree, so I qualified. This act was established as a direct consequence of the Soviet Union's launch of Sputnik I and the perception that the USA was falling behind in science and technology during the Cold War.

I decided then and there to attend Fenn College and accept the scholarship. But a complication arose. It turned out after I decided to attend Fenn, I *was* awarded a New York State Regents Scholarship on the alternates list. I could have gone to RPI where I was accepted but had not been offered financial assistance. Unfortunately, it was becoming too late in the year to change my plans and decided to not to accept it.

During the nearly 5 years I was at Fenn, 1959 to 1964, I was fortunate to be able to hold several part-time jobs during the academic year, which supplemented my co-op earnings. More about the co-op experience shortly. I also worked as one of the operators of Fenn's antiquated PBX telephone switchboard located on the ground floor of Fenn Tower. It was a classic, with long braided wire plugs which had to be inserted into the proper receptacles to connect the outside and inside callers to their desired recipients. I was also employed as one of the operators of the elevators in the Fenn Tower which housed offices, dormitories, classrooms, gymnasium, swimming pool, and book store. I would fill in for the full-time PBX operator and elevator operators (they were "manned" by three women, one for each of the elevator) in the evenings when the evening school was in session and on weekends. Fenn Tower is a 22-story structure originally designed and built to be the ill-fated National Town and Country Club Building in 1929. This gave Fenn College the name "Campus in the Clouds" when it opened in 1938 [2].

If that wasn't enough, at the request of Dr. Frank Bockhoff, Chair of the Chemistry Department, I also worked part time as an assistant in the stock room which served the general and inorganic chemistry laboratories. They were situated in Stilwell Hall, which also held classrooms, offices, a multifunctional auditorium, as well as the library. Stilwell Hall opened in the fall of 1959, the year I enrolled at Fenn as a freshman. The library which had been located on the third floor of Fenn Tower had been transferred to the third floor of Stilwell Hall. Stilwell Hall was spanking new throughout, a $2 million renovation of the old Ohio Motors Building diagonally across from the Fenn Tower on East 24th street. I would dispense chemicals, glassware, and equipment to the students working in these two laboratories. At the beginning of most quarters, I served as part-time help for day and night school registration in several capacities including assistant cashier. During my residency in the dormitory where I lived, I was also a proctor (which either eliminated or defrayed my housing costs) for several of the floors in the dormitory, which was situated, as I remember, on the 11th through the 18th floors of the Fenn Tower. A proctor was a person who was retained by the "house mother" to keep the students on his floor (no females!) under control. The dormitory rooms, which held about 200 men (no women) contained bunk beds, a desk for each student, and were unique in that the single rooms, occupied by two students had their own showers in tiled bathrooms. These dormitory rooms were converted from the guest rooms meant for members of the National Town and Country Club but were never occupied. The exceptions were the end suites which contained two rooms held four to six students who shared the single bathroom. The college provided sheets, blankets, pillows, bedspreads, and drapes and, to top it off, weekly maid service was furnished. These dormitory rooms were originally meant as living quarters for members of the National Town and Country Club. My grade point average may have suffered because of these part-time jobs, but they were enriching experiences. For those interested in the history of Fenn Tower, the Ohio Motors Building, Stilwell Hall, and much more, the reader is encouraged to refer to "A History of Fenn College" [3] authored by Dr. G. Brooks Earnest in 1974, the president of Fenn while I was enrolled there and who presided over the transition of Fenn College to Cleveland State University (CSU) in 1965. I could find no similar comprehensive history of CSU written since the publication of Dr. Earnest's book in spite of its celebrating its 50th anniversary in 2014. Consequently, I had to resort to searching the Internet using Google for information.

Fenn College officially became CSU on September 1, 1965, with the School of Engineering named the Fenn School of Engineering [3]. I graduated in 1964 the second to last year degrees were granted by Fenn College, the last graduating ceremony being June 13, 1965. In 1967, CSU awarded diplomas to graduates from Fenn College, so I can claim I have two undergraduate diplomas, one from Fenn College and one from CSU.

By the late 1990s, Fenn Tower was only housing administrative offices. It was closed in 2000 and slated for demolition. In 2004, the CSU Board of Trustees approved entering into a lease with American Campus Associates to develop Fenn Tower into student housing. Fenn Tower was saved, and a $27.7 million bond allowed the conversion into modern two and four student suites [4]. The restored building was reopened in 2006 and has been registered as an historical landmark. Figure 2.1 shows photographs of Fenn Tower before and after the restoration. The inscription "Fenn Tower" is now emblazoned above the renovated entrance.

Fig. 2.1 Fenn Tower before restoration c. 1965 (*left*) and after the 2006 restoration (*right*). Source:https://www.google.com/search?q=Fenn+Tower&rlz=1C1GPEA_enUS315US382&espv=2&biw=1024&bih=677&tbm=isch&tbo=u&source=univ&sa=X&ved=0ahUKEwiI1vqVjOLNAhVCWSYKHUbuBksQ7AkIQA&dpr=1

Donald Washkewicz, president and chief executive officer of Parker Hannifin Corporation and his wife, Pamela, gave $5 million, and the Parker Hannifin Foundation provided $5 million to CSU [5]. The gift, which equaled the largest in CSU history, went toward scholarships and renovations to the 1920s Stilwell Hall building that housed the Fenn College of Engineering. In November 2013, CSU Trustees then voted to rename the Fenn College of Engineering the Washkewicz College of Engineering. Shortly thereafter, Stilwell Hall was renamed Fenn Hall ensuring that the name of Sereno Peck Fenn, one of the founders of Sherwin-Williams Company [2, 3, 6], past President of the Cleveland YMCA, and benefactor of the YMCA Educational Program, the predecessor of Fenn College, would be enshrined in addition to Fenn Tower.

In addition to engineering, mathematics, and science courses taken while I was at Fenn, I took a generous number of humanities courses. These courses included three quarters of English composition, courses in psychology, sociology, US history, English literature, classical mythology, and music appreciation! Fenn's Music Department consisted of precisely one person, Dr. Julius Drossin, who would supply students of his music appreciation class, on a first-come-first-served basis, 50 cent tickets for the Cleveland Orchestra which at that time was led by George Szell. I believe it was the three courses in English composition which helped me in writing my work reports required for the Cooperative Training Program. The total six quarters of courses work alternated with the total of twelve quarters of classes over a 5-year calendar period. I was fortunate to gain employment with Arthur G. McKee & Company. When I worked there, the headquarters were located at 2300 Chester Avenue, right next door to Stilwell Hall. To get to work, all I had to do was take the elevator down from my dormitory room in Fenn Tower and walk to the main entrance. All of my co-op work was with McKee which proved to be an extremely valuable experience in future years.

When I read these reports now, I am amazed at how detailed and polished they are. The coordinator to whom these reports were submitted graded them, and they all got “A” grades which did not show up on my transcript. What follows is the beginning paragraph from my very first cooperative work report covering a two-quarter period after the first consecutive three quarters of classes in 1964–1965.

> This, my first Cooperative work report period at Fenn, began on the morning of June 29, 1960, at the Arthur G. McKee & Co. As I remember, the day was rather warm and sultry as I approached the revolving door at 2300 Chester Avenue. It was a day which foreshadowed many more to be much warmer, and indeed, much more sultry. With resolution, I pushed through that revolving door at approximately 7:45 and found a cool feeling washing over me as I glanced about me. Seating myself along with several others who had arrived before me, I awaited the receptionist’s arrival. [7]

While at McKee I sat in the “bull pen” with the other co-op students at a collection of desks on one side of a broad hallway around the corner from the Process Engineering Department. Most of the roughly two dozen process engineers had their offices in two rows of cubicles having metal partitions with windows between them. The supervisor and presumably more senior process engineers had their offices facing the rows of cubicles with windows facing Chester Avenue. The bull pen had no partitions between the desks and was located directly across the broad a hallway from two draft persons, one a man and one a woman who sat at their drafting tables. These two draft persons served the Process Engineering Department. Upon occasion, I would be called upon to do some drafting which I did at one of the spare drafting tables preparing flow sheets. Other times I would work in the basement helping an elderly gentleman assembling documents into loose leaf binders bound with metal posts. These books were more than likely operating manuals for the plants designed by the process engineers. My most interesting job, however, was working with an engineer who was performing calculations of pressure–enthalpy relationships for various chemicals produced in the plants designed and constructed by McKee. These calculations were performed by him on McKee’s Burroughs 205 mainframe computer using a program written by the engineer. I was assigned to draw up these pressure–enthalpy diagrams from the computer printouts and to rewire boards inserted into the computer. The computer’s memory was stored on a huge rotating magnetic drum in one cabinet and data stored on a separate console having revolving strips of magnetic tape. This computer, installed at McKee around 1960, was shared through an agreement with Fenn and was used in the computer technology course which I took the last quarter in my senior year.

In April, 1964, the chemical engineering senior student research presentations were held at Fenn where I presented the results of what amounted to my B.Ch.E. thesis research, “Azeotropic Pressure-Composition Investigations” [8]. I then traveled from Cleveland to Terre Haute, Indiana, to the 14th Annual Mid-Central

Regional Meeting of Student Affiliates ACS held at Rose Polytechnic Institute (now Rose-Hulman Institute of Technology); I traveled by plane, for the first time in my life, on a propeller-driven DC-3 aircraft. The experience making this presentation helped me to polish my presentation given the next month at the American Institute of Chemical Engineers (AIChE) sponsored North Central Regional Student Chapter Meeting held at Fenn College. These presentations were the result of my investigation performed in the course chemical engineering research. My advisor was the Chemical Engineering Department Chair at the time, Dr. John T. Cumming. I ran a Colburn still and built my work on the research of a prior student who had worked on this problem but failed to satisfactorily document his results. My objective was to duplicate and extend his results definitively. Each morning I would carefully calibrate the solutions for the binary system chloroform hexane which I was studying. To my astonishment, I was awarded first prize. As I remember it, the then President of AIChE, Donald Dahlstrom, was present at this meeting and congratulated me. AIChE headquarters notified me by letter that I was to receive a year's subscription to the AIChE Journal and a certificate. My win may have chagrinned another member of the Chemical Engineering faculty, Professor Elmore S. Pettyjohn whose student he advised failed to win first prize. More will be related about Professor Pettyjohn in due course.

2.1 Elmore S. Pettyjohn, Former Director of the Institute of Gas Technology, is on the Faculty of the Fenn College Chemical Engineering Department

I took two quarters of unit operations and one quarter of chemical equipment design taught by Professor Pettyjohn and two quarters of unit operations laboratory supervised by him. I remember clearly that during the summer quarter of 1963, the unit operations laboratory was so hot that everyone retired to the bar at the Libido Restaurant and Lounge on the corner of Chester Avenue and East 24th Street. In the class room wherein his courses were taught, instead of the usual chairs, we sat on high stools, which were none too comfortable, at what appeared to be drawing boards, similar to those used in the graphics course classroom, so that we could perform design calculations and drawings.

Pettyjohn was a rather large man, somewhat portly with a belt tightly cinched around his rather large waist, and had greying hair, severely combed back and parted smartly in the middle. He would precede each class with anecdotes and stories that sometimes consumed most of the class time. During these endless and sometimes humorous rants, he would reveal snippets from his previous employment without giving any details. I recall his saying once that he had decided to retire and so he decided upon accepting a teaching position at Fenn in the Chemical Engineering Department. This gave me the impression that he didn't think too much of his position there. I remember upon one occasion, he described, somewhat misty eyed, a scene where well-dressed pretty colored girls would emerge from some building. Later I would learn that the building he described in his mind's eye was the MECCA a dilapidated overcrowded apartment building that was situated just north of the Institute of Gas Technology (IGT) on West 34th and State Streets in Chicago, on the IIT campus. So, that is about the extent I knew about his background. Another student would refer to him as the "Captain." Perhaps he knew more about his past by talking to him in more detail privately. But I never engaged Pettyjohn in any significant conversations since I was somewhat in awe of him. After Pettyjohn wound his stories down, he would suddenly say in effect, "OK now let's get down to work," and the class would suddenly be aroused from its languor. One time we had to design a pressure vessel based on the intricate and detailed American Society of Mechanical Engineers (ASME) standards manual or another time size a distillation column using the McCabe-Thiele method.

Why am I singling out my experience with Professor Pettyjohn in deference to any other faculty member which made an impression on me, like Professor Frank Bockhoff, Chair of the Chemistry Department whom I considered the best teacher I had at Fenn? Well, there is an ulterior motive on my part. I am convinced that he played a pivotal role in my enrolling at the Illinois Institute of Technology in the fall of 1964 upon graduation from Fenn College in June. What follows now is a summary of the second event in my predestination, the first being the events leading up to my attending Fenn College.

Since Fenn College had no graduate school in 1964, and I wanted to continue my education, I would have to leave for another school that had one. I applied to several colleges and universities including Massachusetts Institute of Technology (MIT), Pennsylvania State University (Penn State), RPI, the University of Rochester, Carnegie Institute of Technology (now Carnegie Mellon University), and IIT. My parents still had not accumulated anywhere near enough savings to pay for my graduate school studies, and so as a back up, I also applied to several companies for employment as a chemical engineer in case I failed receive any financial aid. One of them was B.F. Goodrich Chemical Company, located nearby in Avon Lake. I was invited for an interview at their Development Center in March.

I had garnered an exactly 3.0 grade point average which is not superlative, due in large part to the several part-time jobs I mentioned earlier that I held down while at Fenn. I was accepted at MIT, Penn State, RPI, the University of Rochester, Carnegie Institute of Technology, and IIT. I received offers of a graduate assistantship from the University of Rochester, a half-time research assistantship from MIT, and a third-time teaching assistantship with a stipend of \$175 per month for 9 months plus tuition of \$1,450 from Carnegie Institute of Technology. The only offer of financial assistance I received from IIT was, of all departments, the Civil Engineering Department. C. Fred Gurnham, Professor of Civil and Chemical Engineering, explained in his letter of April 9, 1964, that his department had seen my application because the Chemical Engineering Department had called it to his attention. That department liked my record, but their funds for financial aid were depleted. His group was in a better position because it had received a grant from the Public Health Service. He went on to explain that his program was keyed to the problem of industrial wastes and to the chemical approach to sanitary engineering. All I had to do, to be considered for admission and a grant, because his department already had my application, was to express in a letter my interest in this field. The degree would be in Sanitary Engineering, "…which is recognized as a worthy endeavor for Chemical Engineers." I summarily declined it since I considered Sanitary Engineering be totally outside of my field of interest in Chemical Engineering. In April, I received an offer from B.F. Goodrich for a position at their Development Center at a salary at $625 a month. However, by that time I had decided that I really wanted to attend graduate school. So, I declined their offer and accepted the offer from Carnegie Institute of Technology because it was the best one I had and started to make preparations to travel to Pittsburgh in the fall. I told B.F. Goodrich of my decision and asked if I could be employed for the summer. However, they were unable to do so.

The dormitory rooms at Fenn had no telephones in the rooms for the students. However, each floor had one, and only one, pay telephone. When it rang, someone would answer it, and, if it wasn't for him, then he would yell down the hall for the intended recipient or run down the hall way to his room and inform him that he had a call. I was in the final stages of packing up and planning to leave Fenn for Carnegie Tech in the spring of 1964 with the promise of a summer job offer after graduating in June, which I will shortly describe.

Out of the blue, there was a telephone call for me on the pay phone from a Dr. Richard F. Bukacek, who described himself as the Chairman of the Gas Technology Department at the Institute of Gas Technology (IGT) at IIT. It was taken by one of the students who then contacted me to take the call. I didn't even know that IIT had such a department, and I certainly had never had any prior correspondence with the man. I almost hung up on him. I had eliminated IIT from further any consideration after receiving the silly offer from the Civil Engineering Department. Dr. Bukacek proceeded to describe an offer for me to enroll in the Gas Technology Department and proceeded to explain it to me in detail. It was for an IGT Fellowship leading to the degree of a Master of Science in Gas Engineering. This Fellowship would carry a stipend of $335 per month on a 12-month basis amounting to $4,020 per year. He went on to say that this Fellowship ALSO included a full tuition Fellowship. By 1969, IIT full-time tuition for graduate students amounted to $900 per semester. I was stunned since it was better by far than the off from Carnegie Institute of Technology. I estimate that this offer amounted to over $60,000 in 2016 dollars. I hesitated for a few moments and said that if I did accept his offer, I would have to decline the Carnegie Tech's offer after having accepted it and withdraw from enrolling. So, we agreed I would accept the offer contingent upon receiving permission from the Chemical Engineering Department at Carnegie Tech to do so. I received the IGT Fellowship offer in writing and proceeded to contact the appropriate official at Carnegie Tech. I delicately as possible described the situation, and the permission was granted. I then accepted Dr. Bukacek's offer of the IGT Fellowship, and since I had already applied to IIT, I assumed that he would inform the Graduate Office of my decision.

Thus, the second event in my predestination that propelled me to meet Dimitri Gidaspow and Charlie Solbrig was accomplished. The first event has been described earlier concerning the path leading to my attending Fenn College. But what precipitated this incredible out of the blue, so to speak, opportunity to be offered to me? It certainly wasn't any action on my part. My explanation for it will shortly be explained.

Before entering the Gas Technology Department at IIT, I was lucky to obtain a job working the summer of 1964 at the Durez Plastics & Chemicals (aka Durez) in North Tonawanda, New York, which became a part of Hooker Chemical Corporation in 1955. I had interviewed at Hooker while at Fenn and that is how I got the job at Durez. I had taken a night course in polymer chemistry taught by Dr. Frank Bockhoff, Chair of the Fenn College Chemistry Department. This course was sponsored by Arthur G. McKee & Co. and was made available for their employees. I got an "A," but this course never was recorded on my official resume for which I expressed disappointment. Because of taking this course, I became quite interested in polymer chemistry and expressed this information and desire to Hooker and that is how I landed up at Durez. By the time I joined Durez, it was the largest independent manufacturer of phenolic resins and molding compounds in the world. They also manufactured Hefron polyester resins and Hetrofoam, a rigid urethane foam. This facility manufactured phenol which was subsequently used in the production of these phenolic resins. I worked at a variety of positions at the phenol production facility including the laboratory which supported the distillation units that separated the monomer phenol from the chlorobenzene reaction side products. I also worked in the office performing miscellaneous calculations like designing pipe hangers for the piping which conveyed various chemicals.

As I mentioned above, when I was at Fenn, I had no knowledge of Elmore Pettyjohn's past. I had to piece it together during the research for this book. Fortunately, I found out the existence of a book that traced the history of the Institute of Gas Technology's first 50 years written by one of its employees, Wilford G. Bair [9], which proved to be very enlightening. Other details about him were obtained from the Internet. It turns out he was a former Director of the Institute of Gas Technology before he joined Fenn College! IGT was founded in 1941 and was selected to be situated in Chicago on the campus of IIT in May of that year. IGT's early history is recorded in Bair's book [9] to which the reader is referred.

What follows is a brief summary of Pettyjohns's 10-year tenure there obtained from Bair's book. IGT's Trustees selected Elmore S. Pettyjohn born in 1897, as Director Designate in 1945, but because he was still serving in the US Navy, he was unable to assume full control immediately, and Leon J. Willien served as IGT's Acting Director for a year. After receiving his Bachelor's and Master's degrees in Engineering from the University of Michigan in 1922, Pettyjohn spent 5 years in blast-furnace and coke-oven operation in Chicago. He subsequently held various positions within the gas industry for the next 13 years, as well as teaching at his alma mater. As a naval reserve officer from World War I, Pettyjohn was called to active duty in 1940 and served throughout World War II. He was discharged as a captain in 1946, when he joined IGT as Director in May. This is clearly the reason some students and perhaps even faculty at Fenn referred to him as "captain." One of his first priorities was to establish a new building to house IGT. He was responsible for raising funds for construction of this two-story building which had to conform to the style developed by Mies Van der Rohe, the architect of the IIT campus at the time. It was built on the southwest corner of West 34th and State streets in 1949. It housed offices, classrooms for the Education Department, research laboratories, and the library. Pettyjohn directed IGT for 10 years, becoming Vice President and Director in 1952. IGT grew substantially under his leadership. However, questions were raised by the Board of Directors at the December 1954 meeting of IGT's Executive Committee concerning the relationship between the American Gas Association (AGA) and IGT. It was felt that IGT was not receiving adequate funding for utilization and distribution system research and that this funding could be increased by improving IGTs relations with AGA headquarters staff. A study was made to assess this relationship, and the report was submitted to the Executive Committee in November of 1955. The nature of the recommendations made in this study was not revealed in the record of this meeting. Pettyjohn resigned as Director the following morning at the Annual Meeting of IGT members. He stated that he had planned to come to IGT to serve a 5-year term and that although the job of getting the institute organized had taken twice as long as he anticipated, he considered that his work at IGT, now in the middle of its second decade, was now finished. Dr. Henry R. Linden, who would later become Director and President of IGT for nearly 30 years, became Acting Director until Dr. Martin A. Elliot became Director in 1956.

It seems clear to me by reading between the lines contained in Bair's book that something serious had been unearthed by the IGT Executive Committee report, thus creating a cloud of suspicion over Pettyjohn's behavior which resulted in his precipitous resignation as Director. It is not clear how long Pettyjohn remained on at IGT after resigning. He joined Fenn's Chemical Engineering Department in 1958. As I mentioned earlier, he stated in his classroom stories that he had "retired." He would have been only 61 years of age when he started at Fenn being born in 1897. By 1963–1964, when I took his unit operations and chemical process design courses, he was in his middle 1960s, and his hair was already mostly gray as shown in Fig. 2.2 taken in Fenn's unit operations laboratory.

Pettyjohn retired from Fenn in 1968. I drove to Cleveland from Chicago to help celebrate his retirement. I forget just how many of his former students, chemical engineering, and other Fenn College department faculty attended. As I recall, one of his students who cooped at Arthur G. McKee & Co. with me, Russell Sage, who graduated with me, was hired by the company after he graduated and remained in the Cleveland area. He helped to organize Pettyjohn's retirement party and was the one who contacted me about it. After the party, I attempted to find accommodations at the Cleveland YMCA a couple of blocks from Fenn. Since it was full, I drove back to Chicago!

Here is my explanation for Dr. Bukacek's infamous telephone call to me in 1964 offering me that generous IGT Fellowship. I am convinced that Pettyjohn

Fig. 2.2 Professor Elmore S. Pettyjohn in Fenn College Stillwell Hall unit operations laboratory. Photograph courtesy of Bill Becker, Cleveland State University Archivist

recommended me to Dr. Bukacek as being a good candidate for an IGT Fellowship. I didn't apply for it and I didn't know such a Fellowship existed. I got one "A" and the rest "B's" in Pettyjohn's courses and graduated as a "B" student with an exactly 3.0 grade point average. It's not a likely I would have gotten the Fellowship if I applied for it, which I didn't. Thus, the moving finger from Chicago plucked me from Cleveland and landed me squarely in the presence of Gidaspow and Solbrig in the Gas Technology Department at IGT! The next Chapter will chronicle my experience there in the years 1964 to 1970.

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Chapter 3
Illinois Institute of Technology (IIT), Chicago 1964–1970

With my savings and with some help from my parents, I bought a new 1964 Corvair costing about $2000 during that summer after I arrived back in Dunkirk from Cleveland. I used this automobile to hone my driving skills (I took driver education in high school) by commuting alternate days with an employee of Durez who happened to also live in Dunkirk. North Tonawanda is located north of Buffalo about 50 miles from Dunkirk. Most of the driving was on Interstate 90, but even then the other employee and I had to get up quite early in the morning to arrive in time to start work at 8:30 am. I used this new Corvair to drive to IIT from Dunkirk to Chicago in the fall of 1964 after completing my employment at Durez.

This wasn't the first time in Chicago for me, but I had never before stepped onto the IIT campus. Three or four classmates from the Chemical Engineering Department at Fenn, including myself, traveled by car from Cleveland to attend the 1962 AIChE Annual Meeting held in Chicago December 2–6. This was in the days before the Interstate Highway System was completed connecting Cleveland and Chicago, which would reduce the daylong trip to about 6 h. The department provided subsidization for gasoline, registration, meals, and housing accommodation. I think we stayed at the Chicago Hilton, the venue for the meeting. Upon arriving in Chicago heading to the downtown, I clearly remember the long row of high-rise buildings alongside the Dan Ryan Expressway. I later learned that this collection of high rises, terminating just south of IIT at 35th street, was the Robert Taylor Homes project completed in 1959. It housed low-income residents, almost entirely blacks, which were displaced by extensive slum clearance of condemned and abandoned buildings, called Bronzeville, and construction of the Dan Ryan. Bronzeville, aka the South Side of Chicago or the Black Belt, extended from 22nd to 63rd streets between Wentworth and Collage Grove [1]. Between 1942 and 1944, the black population reached 337,000, one-tenth of Chicago's total. While I was at IIT, the Robert Taylor Homes buildings began to turn into high-rise slums with gang wars, drug pushers, and frequent homicides. They were subsequently completely demolished by 2005. It was quite an experience at the meeting seeing, walking around in the flesh, famous (to me anyway) chemical engineers I read about in our

R.W. Lyczkowski, *The History of Multiphase Science and Computational Fluid Dynamics*, Mechanical Engineering Series,
https://doi.org/10.1007/978-3-319-66502-3_3

chemical engineering text books and journals, such as James Knudsen and Stuart Churchill.

The first thing I did was to obtain my dormitory room assignment by checking in with the Housing Office located in the Commons building erected in 1954 [2]. In the 1960s, this building also held a grocery store, post office, cashier, dry-cleaning shop, book store, medical offices, cafeteria, and a barber shop [3]. The mainframe computer was located in the basement. It was an IBM 7040, later replaced by an IBM 360/40/2702, which was replaced by a UNIVAC 1108 in 1969. Graduate students were housed in Fowler Hall, a four-story residence (as were all the dormitories) built in 1948 [2]. Undergraduate students were housed in Farr Hall also built in 1948, and in the North and South wings, constructed in 1959. None of these dormitories were air-conditioned. The East wing was added in 1965 to accommodate the increased undergraduate enrollment. In 1966, graduate students could relocate to the new Graduate Hall, and women were housed in the new Women's Hall. Before this, there were no women students in the campus dormitories. All freshmen students and undergraduate women students were required to live in the campus residences unless they lived at home or with relatives [3]. Except for Farr Hall, these six residences are connected to one another and to the central dining room and lounge. Twenty-one meals per week were included in the dormitory accommodations for the academic year from September to June, most of which were double occupancy. Single-occupancy rooms were only available to graduate and woman students residing in the graduate and women's wings which were air-conditioned. The four high-rise apartment buildings (dates refer to their year of construction) [2]: Gunsaulus Hall (1949), Carmen Hall (1953), and Bailey and Cunningham Halls (both 1955), housed married students. Gunsaulus Hall was the first apartment building built on the IIT campus named for Frank Gunsaukus, the first President of Armour Institute of Technology (AIT). In 1941, AIT merged with Lewis Institute to form IIT. Students could also be housed in the apartment buildings which were more expensive than the dormitories. Many undergraduates elected to live in the nine fraternity houses built between 1959 and 1962.

Having been living in relative splendor in the Fenn Tower in Cleveland which had individual bathrooms and showers in each double-occupancy single room, my first shock upon surveying my new dormitory room in Fowler Hall was that there was only a single community bathroom with showers for the entire floor. And like Farr, North, and South dormitory Halls, it was not air-conditioned, but neither were the dormitories in Fenn Tower. The rooms in Fowler Hall were furnished with bunk beds, desks, and enough room for bookshelves. Addition storage was supplied in the basement which contained a recreation room. Coin-operated washing machines and dryers were located in the basement connecting North and South Halls. Free parking was available in the adjoining lots southeast of the North and South Halls between Wabash Avenue, west of State Street, and north of 33rd Street. A fee was charged for access to a small fenced-in parking lot located south of the Service, station built in 1960, with a keyed padlock for added security. Since my car was quite new, I paid for this option.

I stayed in Fowler Hall for only one or two semesters where Frank Kulacki was resident advisor. He had started as a graduate student in the Gas Technology Department at IGT in 1963 after graduating in just 3 years from IIT with a B.S. in Mechanical Engineering and a minor in Gas Engineering. It took Frank just 3 years to get his B.S., but 3 years to earn his M.S. in Gas Engineering in June 1966. We struck up a great friendship during the time he was at IGT. He left for the University of Minnesota to do his doctorate. After graduating in 1971, he entered academic life, teaching at Ohio State University, the University of Delaware, Colorado State University, and eventually at his alma mater, the University of Minneapolis where he is now a Professor in the Mechanical Engineering Department. His wife Jane is also a professor at the University of Minnesota. Frank and I have remained lifelong friends.

With Frank's encouragement, I applied for an opening for the position of resident advisor in the North Hall. I explained to the Dean of Housing that I had experience as a proctor in the dormitories at Fenn College. I was successful in obtaining this position which I occupied until I graduated in January 1970. The position provided for a furnished two-room apartment on the first floor of North Hall. The larger of the two rooms had a telephone, window air conditioner, a foldout sofa bed, a kitchenette, and, lo and behold, a bathroom with a shower (shades of Fenn). There was a door connecting to the smaller of the two rooms, which I used as a store room instead of an office since I had one at IGT. In lieu of salary, the apartment was provided free of charge as were meals in the dining room for the entire calendar year. Consequently, I now had no expenses to speak of so my IGT Fellowship allowed me to actually accumulate some savings which were deposited in a nearby bank and the remainder provided for miscellaneous expenses. These included car insurance, licenses, gasoline, and maintenance for my car which provided travel around the Chicago area for an occasional get together with classmates in places such as the Old Town bars and restaurants, Siebens's Brewery, and the like.

After settling in at my dormitory room in Fowler Hall, I went to meet with Dr. Bukacek, Chair of the Gas Technology Department, and to be shown to my office accommodation. The Department of Gas Technology was part of the Education Division in the Institute of Gas Technology (IGT). The Department offices were housed on the second floor of the IGT building, which construction began in 1949 on the corner of 34th and State Streets and eventually completed and occupied in 1950 [4]. Remarkably, the building was air-conditioned equipped with an absorption lithium chloride/lithium bromide absorption cooling system. Other campus buildings constructed just prior to the IGT building in 1946 (Alumni Hall) and 1947 (Perlstein and Wishnick Halls) [2] were not air-conditioned. They had to be retrofitted with non-protruding-window air conditioners in the offices and laboratories so as to not ruin the esthetic qualities of the Mies-designed building exteriors. The second IGT building, which was added in 1964, did not yet exist. The library, Director's Office, drafting room, and two classrooms were also on the second story, which had no elevator access. There was a freight elevator toward the back of the building used exclusively for moving laboratory equipment and heavy loads. Anecdotal stories related to me were that Pettyjohn insisted during the building's design that no elevator was be installed ("Why, it's only two stories, you can walk up!") and that the non-opening windows were to be located high in offices and laboratories next to the ceiling so that nobody could peer idly out of them. Several laboratories, the Industrial Education Department offices, and the precision machine shop were located on the first floor.

There were two rooms in the basement of the building, which were provided to the Fellowship graduate students as office space. One room for the students was partially outfitted with two private offices, desks, and shelving. Four more desks were situated immediately outside of these two offices but in the same room. These four desks were more or less partitioned from each other and were quite cramped, allowing little room for storing books, papers, and personal belongings. In an adjacent room, there were provided desks, shelving, and furniture stored there, cast off from the IGT staff. I had my desk in the first room outside the private offices, which were already occupied by one M.S. candidate Claude H. Traylor and one Ph.D. candidate, Joseph P. Dolan. In the years I was a student at IGT (1964–1970), there were roughly a dozen graduate students occupying these two rooms. There were also several more laboratories, the printing shop, and the computer room in the basement.

There was one other Ph.D. candidate which I will single out now by name, because of his playing a signal role in my career and his role in the history of multiphase science and computational fluid dynamics, was Charles W. Solbrig. He was known as "Chuck" by his colleagues and "Charlie" by his family and Chicago connections. I will subsequently refer to him simply as Charlie. He was born in Chicago in 1938. His father was a medical doctor who had a practice in the basement of the house where his parents and two brothers lived. His father owned the von Solbrig Hospital located on Chicago's south side [11]. Charlie went to St. Nicholas grammar school and graduated from Mount Carmel high school excelling in mathematics and physics. Charlie then enrolled at IIT in the Mechanical Engineering Department. He was offered a scholarship by the Institute of Gas Technology for his junior and senior years. During the summer of 1959, he was hired by IGT and worked as a technician helping Dimitri for his doctoral research on surface combustion of hydrogen [6]. Later that summer, Charlie married his wife Carol and eventually had four children, three girls and a boy. Charlie received his B.S. in Mechanical Engineering in 1960. He then enrolled as an IGT Fellow to pursue his graduate studies and earned his M.S. in Gas Engineering in 1962. Charlie's thesis involved the experimental determination of the compressibility of hydrogen–methane and hydrogen–ethane mixtures over a wide range of pressures and temperatures in the IGT Fluid Properties Laboratory. After his graduation, he left the Department of Gas Technology for two and one half years from 1962 to 1964 to work at the Armour Research Foundation (ARF), changed to IIT Research Institute (IITRI) in 1963, located in the five-story building located on the corner of 35th and State Streets just one block south of IGT. This building was demolished after the 20-story IITRI Research Tower was erected in 1965. While at ARF/IITRI Charlie did research on a turbine compressor, a multifuel diesel engine, a smokeless oil burner, thermal radiation, and measurement of explosion limits in space simulation chambers [5]. During these two and one half years, he continued to take graduate courses and finished the needed Ph.D. course work at night. With two weeks preparation, Charlie took the three-day written comprehensive examination with two other Ph.D. candidates who had taken a year to study for it. One was asked to leave the program and one did so well that he was able to skip the oral examination. Charlie passed the comprehensive examination and was required to take the oral examination. After several failed attempts to line up a sponsored project at ARF and the encouragement of Dimitri in the Gas Technology Department and his agreement to be his advisor, Charlie then returned to IGT as a full-time graduate student in 1964 to pursue his doctorate. Perhaps as a result of his experience at IITRI and the current research interest of Dimitri, Charlie became his very first successful Ph.D. student and embarked on his thesis the study of convective diffusion with surface reaction in both laminar and turbulent flows. This was to be a purely analytical study because of Charlie's experience in the IGT Fluid Properties Laboratory, which had to be evacuated because of an accident whereby mercury liquid and vapor were released from an extremely high-pressure apparatus, thereby contaminating the laboratory. Charlie entered the laboratory to shut off the leaking pipe, thus exposing himself to the mercury vapor. Charlie was ensconced in the basement, separate from all the other students in an office which he shared with a defunct, non-operating electron microscope.

3.1 Professor Gidaspow Is on the Faculty of the Gas Technology Department

When I started at IGT in September of 1964, the number of faculty in the Gas Technology Department was quite small [5]. There were only seven graduate students including myself. Dimitri alone taught only IGT graduate courses and graduate courses in heat transfer and applied mathematics in the Chemical Engineering Department. When this was done, the courses carried a dual IGT and ChE course number depending on whether the student was in the Gas Technology or Chemical Engineering Department. He also directed graduate students' research in areas of his interest at the time which included combustion, mass transfer, and heat and mass transfer in fuel cells. Dr. Bukacek was appointed Education Director and Chair of the Gas Technology Department in 1963 following Rex Ellington and was responsible for all of IGT's undergraduate, graduate, and industrial education programs. To complement Dimitri's teaching the graduate studies, Dr. Stuart Leipziger joined IGT's Education Department in 1965 to administer IGT's undergraduate education program, teach both graduate and undergraduate IGT courses, and advise graduate student research projects. So, in 1964, Dimitri was pretty much the sole faculty in the department besides Dr. Bukacek. All three of them had quite recently received their Ph.D. degrees: Dr. Bukacek in Chemical Engineering from IIT in 1960, Dimitri from IGT in Gas Technology in 1962, and

Dr. Leipziger in Chemical Engineering at IIT in 1964. The other members of the Education Division were the Manager of the Industrial Engineering Program, Gerald G. Wilson and a Senior Engineer in charge of Sales Engineering. Several IGT staff also taught graduate and undergraduate courses and advised graduate student research part-time since they did not have sufficient credentials to be full-time faculty members of the Gas Technology Department. These staff members were given titles of Adjunct Professor and Adjunct Associate and Assistant Professors of IIT and were employees of IGT and not IIT. The members of the Gas Technology Department, including Dimitri, were also employed by IGT.

Before continuing with the story of my graduate student experience at IGT, I am now going to present a profile of Dimitri's background in some depth up to 1964, the year I joined the Gas Technology Department, because he plays such a central role in this book's history of multiphase science and computational fluid dynamics. This background will serve to shed some light on the nature of Dimitri's breadth of character. Dimitri was born in 1934 at Kobeliaki (or Kobel'aky), Ukraine, which is southeast of Kiev and south of Poltava. Kobeliaki is on a river where he would frequently swim or bathe. His mother was an entomologist, and his father was an agricultural engineer. They both worked in a rural agricultural experimental station called Veseliy Podol, administered from Kiev. His mother received a medal from Nikita Krushchev for her joint discovery of DDT used to eradicate the insects that devour sugar beet plants. He was educated by his mother and didn't attend grade school until about the age of nine after which he attended several schools for about a year. While his parents worked, he stayed with his grandmother [6]. He learned to read Ukrainian and read and write Russian which would be useful to him in future years. Before the end of World War II, his family moved to Quedlinburg Germany in Saxony which was near the Hartz mountains. This area was being occupied by American soldiers but eventually became annexed by the USSR. One month after the end of the war in 1945, his family moved again, this time to Heidelberg, Germany. There Dimitri entered the Realgymnasium, an eight-year German school specializing in foreign languages and science, which was an alternative to Latin school. He stayed only 3 years. He and his parents then immigrated to the USA in April 1949.

He went to Seward Park high school in New York City and graduated in 1952 as valedictorian of his class. He remembers that his class was truly impressive. He is still friends with a former classmate, Stanley Engesberg who is a physicist. After graduation, Dimitri attended the City College of New York from 1952 to 1956 and worked there for the Registrar together with about a dozen top students who assisted the Registrar to handle the complex logistics of enrolling students in the available classes. One of these students who worked with Dimitri is now a professor at the University of Texas, Austin, but Dimitri cannot recall his name. Dimitri received a BChE degree in 1956 cum laude, at which time he joined the AIChE and is now a member of the select group of 50-year members. In the summer of 1956, Dimitri worked for a month in Allentown, Pennsylvania for Air Products for a Dr. Lapin (Dimitri does not recall his first name) and the research director.

Dimitri applied to IGT's Gas Technology Program in 1956 after graduating from City College, but enrolled instead at Polytechnic Institute of Brooklyn because he felt that it was a better university than IIT. Two of his professors there at the time were Donald Othmer who taught fluid mechanics courses, and Ju-Chin Chu who taught distillation and thermodynamics courses. The reader may not be too familiar with the name of the latter. He is the father of Paul Chu who, in 1987, headed the team that discovered the superconductor which operates at 98 K, which is above the boiling point of liquid nitrogen [7]. In 1997, he shared the Nobel Prize in physics for laser cooling to trap atoms. He became the twelfth Secretary of Energy from 2009 to 2013.

The reader may be more familiar with the name of Donald Othmer. He joined the Polytechnic Institute of Brooklyn in 1932 teaching in the Chemical Engineering Department, becoming the Head of it in 1937 in which capacity he continued until 1961. He became Professor Emeritus in 1976 but remained active in what became the Polytechnic University until his death in 1995. He is also known for establishing the *Kirk-Othmer Encyclopedia of Chemical Technology* in 1945, together with Raymond Kirk, a chemist at the Institute. An interesting connection to Dimitri' education is that Othmer attended Armour Institute of Technology in Chicago as an undergraduate for a brief time, but left for the University of Nebraska, graduating in 1924 with a B.S. in Chemical Engineering. The reader will recall from earlier in this chapter that Armour Institute of Technology (AIT) was the predecessor of IIT.

Dimitri's Master's thesis was titled *Arsenic-Aluminum-Zinc Equilibrium*. His advisor was Professor Schurig for whom he worked 2 years teaching unit operations laboratory. "This was good the first year but slave labor the second". Dimitri graduated from Polytechnic Institute of Brooklyn in with an MChE degree in 1959 and in 1960 he married Helene, his childhood sweetheart in the Ukraine. In 1958, the year before he graduated from Polytechnic Institute of Brooklyn, Dimitri applied to the work-study program established in the Gas Technology Department at IIT by Rex Ellington, then the Director of Education at IGT who had established the Department. Prior to this, the work-study program was part of the Chemical Engineering Department. The students were paid the equivalent of three-fifths of an engineer's salary. IGT had been enrolling students since 1941 with the first M.S. graduating in 1944 and the first Ph.D. in 1946 [4], but there was no IIT Department of Gas Technology [11]. Qualified IGT staff members were appointed as Adjunct Professors, and part-time professors were hired from various IIT departments. Donald Othmer wrote a letter of recommendation for Dimitri to Henry Linden who became Director of IGT in 1961. Dimitri then had an interview with Rex Ellington who was visiting in New York which resulted in his joining the Department of Gas Technology work-study program for the fall semester 1958–1959. There were just three graduate students from colleges and universities other than IIT including Dimitri. The other two were Dan Magasanick, who received his M.S. in 1963, and Kenneth E. Starling, who received his M.S. in 1960 and his Ph.D. in 1962 both from IIT. He and Dimitri were students in the Gas Technology Department at IIT, graduating together with Doctorates in Gas Technology in 1962. Starling joined the Chemical Engineering Department at the University of Oklahoma in 1966 and became Professor Emeritus of the Chemical, Biological, and Materials Engineering Department in 1995. His is known for two equations of state widely used in the field of Chemical Engineering which bear his name: Carnahan-Starling and the Benedict-Webb-Rubin-Starling (BWRS). His hard-sphere equation of state for which he developed the radial distribution function is used by physicists and chemical physicists as a theoretical tool to separate hard sphere from other short-range molecular interactions. Frank Kulacki told me, and Dimitri concurred, that Dan Magasanik eventually went to Australia to found his own energy company.

The Gas Technology Department was not unique. There is a similar one at Pennsylvania State University and one at Telemark Institute of Technology in Porsgrunn, Norway, where Dimitri much later taught a short course. Unfortunately the Department of Gas Technology at IIT, initiated in 1941, was phased out over several years in the 1980s so that students who entered in January 1983 could complete their course work and graduate in an orderly fashion. At that time, a 5-year notice was given to IIT that the academic program would be discontinued and the affiliation between IGT and IIT was officially ended in 1988. The last Ph.D. in Gas Technology, Stephen Folga, graduated in 1987. Then in 1994, IGT moved from the IIT campus to larger facilities in Des Plaines, Illinois.

Dimitri's Ph.D. thesis, *Surface Combustion of Hydrogen* which was primarily experimental, involved the determination of the rate of surface combustion of hydrogen on platinum-coated alumina and oxidized nickel and resulted in two peer-reviewed publications [8, 9]. He started by modifying the apparatus which already existed in a laboratory on the first floor of IGT next to the Fluids Property Laboratory. It was a behemoth with special power lines supplying electricity to heat the tubes upon which the surface-catalyzed reaction occurred at several hundred degrees Fahrenheit. As mentioned earlier, Charlie Solbrig helped Dimitri in 1959 to take reaction rate data for the surface combustion of hydrogen in turbulent flow to eliminate diffusive effects. Dimitri graduated with a Ph.D. in Gas Technology in June 1962. Rex Ellington was his advisor who left IGT shortly thereafter.

After earning his Ph.D. at IIT in 1962, Professor Ralph Peck, then the Chairman of the Chemical Engineering Department, offered Dimitri a teaching position as a Lecturer to which he responded, "Fine. But chances are I won't be in Chicago for long—maybe one year" [10]. During 1962–1963, Dimitri taught two graduate courses, heat transfer and thermodynamics, and two undergraduate courses, thermodynamics and numerical methods. In addition, he advised Dr. Peck's graduate students, while he was away on his sabbatical. After this teaching experience, Dimitri looked for an industrial position. His best offer was a position in the DuPont Central Research laboratory. "At that time it was the best chemistry laboratory in the world. But IGT offered me the same high salary as DuPont and a Ph.D. candidate. So I went back to IGT. The first year at IGT was challenging" [11]. Dimitri was appointed as an Adjunct Assistant Professor in 1963. His first Ph.D. candidate failed to pass his qualifying examination and was powerless to help him [6]. In a year the situation improved when he began working with the late Bernard Baker (whom everyone including Dimitri called Bernie) on fuel cells, and in 1964 Charlie

Solbrig became his Ph.D. student. Dimitri was also teaching again in the ChE Department and taught applied mathematics and heat transfer [6].

3.2 Charlie Solbrig Is on the Faculty of the Gas Technology Department

Early in 1965 I was assigned to a basic research project, initiated before I joined IGT, which involved thermal analysis of a fuel cell battery. This was my work-study assignment for my special research and problems course. I helped Dimitri to do some of the calculations which he was working on together with Bernie Baker, then Manager of IGT's Energy Conversion Research. Next I was assigned to assist Charlie Solbrig to do some calculations for him as part of his Ph.D. thesis which he was pursuing in 1964–1966. These calculations, as well as the ones for Dimitri, were performed on IGT's IBM 1620 mainframe computer conveniently located between Charlie's office and mine in the IGT basement. The IBM 1620 was the second of IGT's computers installed in 1961 [4] and was one of the earlier models introduced by IBM in 1959 [12]. The first was an ALWAC III built by Logistics Research, Inc., purchased in 1955, and was a behemoth which consisted of vacuum tubes and diodes and cost in the vicinity of $80,000 [4]. According to Dimitri, this was the first mainframe computer installed on the IIT campus [6]. The ALWAC was one of the first computers in the gas industry and was used primarily to compute network flow in gas distribution systems. The IBM 1620 was much more compact because it was a solid state machine using transistor technology.

Charlie obtained his Doctorate in January 1966 with his thesis *Convective Diffusion In a Rectangular Duct With One Catalytic Wall*. He then promptly joined IGT and obtained an appointment in the Department of Gas Technology as an Adjunct Assistant Professor along side Dimitri and Stuart Leipziger. Working with Charlie on his Ph.D. thesis proved very stimulating to me, and so Dimitri and I discussed extending a portion of Charlie's thesis to analyze convective diffusion of the product of reaction for my Master's thesis. Dimitri became my advisor and Charlie became my co-advisor while he was working on his Ph.D. thesis, for which Dimitri was his advisor. This was a bravura act on Dimitri's part! In addition to performing computations on IGT's IBM 1620 computer, I also performed some experimental work in Dimitri's old laboratory where he had performed his Ph.D. investigation on the surface combustion of hydrogen. The apparatus he constructed, which held tubular reactors, had been dismantled and completely removed. In 1965–1966, Frank Kulacki, another IGT Fellowship student who started in 1963 the year before I did, designed and built an entirely new apparatus having a rectangular duct with one reactive catalytic wall. He used it for his Master's thesis with Dimitri as his adviser. This made it easy for him to replace the reactive section without dismantling the entire apparatus. Frank's thesis had as its objective the experimental determination of the rates of catalytic combustion for hydrogen and methane.

My objective was to compare experimental results for the catalytic combustion of hydrogen and the product of combustion, water vapor, with the analytical results Charlie and I had performed. I finished my thesis *Convective Product Diffusion—An Extended Graetz Problem* and graduated with an M.S. Gas Engineering in June 1966. I was encouraged by Dr. Bukacek to apply to the American Gas Association for a Fellowship in Natural Gas Technology for the academic year 1967–1968. I did so and included a copy of my M.S. thesis. I was awarded this Fellowship of $2000 which allowed the AGA to pick up this amount for my IGT Fellowship stipend. Frank also finished his M.S. Gas Engineering in June 1966 with his thesis *Catalytic Combustion in a Flat Rectangular Duct*. His experimental results for the catalytic combustion of hydrogen in laminar flow were used to compare with the analytical results computed by Charlie in his Ph.D. thesis. Frank then decided to leave IGT and went to the University of Minnesota to do his Ph.D. in heat transfer, and I decided to stay on at IGT to do the same.

In 1967, Bernie Baker, who by then had risen to be IGT's Assistant Director Energy Conversion Research, was awarded a two-year contract to model fuel cells for the then-proposed manned orbiting laboratory (MOL) space station for the National Aeronautics and Space Administration (NASA) Astrionics Laboratory, Huntsville, Alabama, the Director of which at the time was Wernher von Braun. The fuel cell proposed to be utilized was to be the one developed by Allis-Chalmers which had an immobilized aqueous potassium hydroxide (KOH) electrolyte and used used ultra-pure hydrogen and oxygen. These reactants were introduced into dead-ended anode and cathode chambers because of the method of water removal via another KOH plate using the vacuum of space. The timing of this contract, from June 1967 to June 1969, couldn't have worked better for Sarvajit S. Sareen from the Chemical Engineering Department at IIT and me. We both were to work for our Ph.D. theses on this contract headed by Bernie. We became Dimitri's next two Ph.D. students after Charlie who began serving as my co-adviser.

For structural rigidity, desirability to have current collectors contacting the electrodes, and the necessity to remove heat by conduction, Allis-Chalmers designed the gas compartments with a complex internal structure [13]. Sareen's thesis involved the difficult task of measuring the pressure profiles in a typical Allis-Chalmers fuel cell. He was able to show that Darcy's law could be used in two dimensions to determine the permeabilities, one for the main flow direction and the other perpendicular to it. The flow in the third direction normal to these two flows is extremely low because of the thinness of the flow channels. This is the reason the analysis can be performed in two dimensions. Consequently, the basic idea was to treat the flow in the gas compartment using a porous media formulation. In effect, this is a highly simplified two-phase model wherein the solid phase, the flow compartment internals are rigid, and the second phase is the gas. This model makes it practical to compute the flow in the highly complex flow paths. Sareen tried, but even today with massively parallel high-performance computers, would require millions of mesh points and long computation times.

My Ph.D. thesis involved the one- and two-dimensional computations for the Allis-Chalmers fuel cell with reaction resulting from current generation. I used the permeabilities measured by Sareen. The one-dimensional model was solved on IGT's small IBM 1800 computer. However, the two-dimensional problem had to be solved on IGT's IBM 1620 and IIT's IBM 360/40/3702 mainframe computer which was much faster. Another objective of my thesis was to experimentally determine the dynamics of moisture removal and to measure the effective diffusivity of water through a KOH-soaked asbestos matrix.

My thesis was *Transport Process in Fuel* Cells and Sareen's was *Fluid Dynamics in Fuel Cell* Cavities. We both graduated in January 1970, Sareen with a Ph.D. in Chemical Engineering and I with a Ph.D. in Gas Technology. Dr. Peck was also Sareen's advisor. Our contributions and those of IGT staff as well as one Master's student from Japan are summarized in the Final Report [13]. During this project, in 1959 Bernie earned his Ph.D. in Chemical Engineering with Dimitri as his Ph.D. thesis advisor at IGT and Darsh Wasan as his advisor from the Chemical Engineering Department. This would not be the last time Dimitri would advise his supervisor. In September, 1970 a Certificate of Appreciation was sent to all of the contributors signed by Wernher von Braun. I can truly say that the five and one half years I spent at IGT taking courses from Dimitri and Charlie and having them as advisers for my two theses was a truly memorable experience. My grades were considerably better than at Fenn college due to the fact that I held no part-time jobs and the semester system was less hectic for me then the quarter system at Fenn.

Let us now recount the number of events so far which, if they did not occur, I would not be writing these lines: 1. I enroll at Fenn College instead of a college in New York because of a late receipt of a New York State Regents Scholarship. 2. I place first in paper presentations at the AIChE North Central Regional Student Chapter Meeting. 3. Elmore S. Pettyjohn, former Director at IGT, is on the faculty of Fenn's Chemical Engineering Department. 4. Dr. Bukacek, Chair of the Gas Technology Department at IIT, telephones to offer me an IGT Fellowship with full tuition. 5. Dimitri decides to pursue his Ph.D. at IIT. 6. Dimitri decides to join IGT Gas Technology Department after obtaining his Ph.D. rather than accept employment at DuPont. 7. Charlie Solbrig becomes Dimitri's first successful Ph.D. student. 8. Charlie decides to join IGT after obtaining his Ph.D. and becomes co-adviser for my Master's thesis.

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Part II
In a State Far Away 1970–1977

Wherein is told of the formation of an effort to develop an entirely new computer program (code) to analyze the safety and licensing of water-cooled nuclear reactors.

Chapter 4
The Seeds Are Sown by Larry Ybarrondo and Charlie Solbrig in a State Far Away, Idaho Falls, Idaho

In my paper [1], I characterized the time span 1970–1977 as **The Initiation Phase. Idaho Falls, 1970–1977**. At that time I had no idea as to the true story of what circumstances made it possible for what I will refer to as *the SLOOP Code project* to be initiated at Aerojet Nuclear Company (ANC) by Charlie Solbrig. Because of the gracious help of Larry Ybarrondo and Charlie, this part of the story can now be fleshed out. When I wrote that paper, I also did not know of the diabolical effort on the part of one individual at the NRC, whose name will shortly be revealed, to deliberately destroy this project. This destruction was totally independent of any of the incredible pioneering scientific merits of the SLOOP Code. The investigators working for Charlie, including myself, were never told of this plot. If it had been revealed, I am sure we would have scattered early on and nothing would have been produced. This distasteful miscarriage of the politics of science can now be revealed for the first time due to Charlie's revelations forthrightly passed on to me.

As I mentioned briefly in Chap. 3, Charlie started to serve as coadviser for my Ph.D. thesis when Bernie Baker was awarded a contract with NASA in 1967. Charlie harbored the desire to obtain numerical solutions of the continuity, momentum, and energy equations for single-phase flow which led him to search for an opportunity to pursue such work not available at IGT. Toward the end of 1968, as Charlie's wife Carol was about to give birth to their fourth child, a son, an opportunity arose at Westinghouse Electric Corporation in Pittsburgh for a position managing a group of analysts developing nuclear reactor safety computer models. Unbeknownst to Dimitri, his former thesis advisor, and fellow faculty member who by now was promoted to Adjunct Associate Professor, Charlie had applied for this position. As Dimitri related it to me [2], Long Sun Tong at Westinghouse woke him up one morning with a telephone call as a reference for Charlie's job application. Dimitri and Charlie had been collaborating on writing a proposed book on numerical techniques, and Tong was asking Dimitri a lot of questions about it. Tong must have been sufficiently impressed by Dimitri's recommendation for Charlie and so was offered the position. He accepted the offer, left the Department of Gas Technology in late 1968, and joined Westinghouse as Manager of the Scientific

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Programming Group. Long. Sun Tong, author of the well-known text on boiling heat transfer [3], was at that time Manager of Thermalhydraulic Engineering for commercial pressurized water reactors (PWRs) at Westinghouse and thus became Charlie's supervisor.

The power output of commercial PWRs is limited by the possibility of the heat flux in the reactor core exceeding the critical heat flux (CHF). This is termed burnout, or departure from nucleate boiling (DNB) [3]. Why is this important? Nucleate boiling is a very efficient form of heat transfer. Once CHF is exceeded because of a decrease in heat flux caused by steam blanketing, the path from the incoming liquid water DNB will occur, and the fuel rods will experience a rapid temperature increase which could result in cladding failure and reaction with steam so as to produce hydrogen. Tong was considered an expert on this subject because of his book written in 1963 containing his CHF correlations. Westinghouse valued him because it was he who determined the conditions which ensured that their nuclear reactors would not experience DNB while operating at their licensed power output. This made it possible for their PWRs to be licensed in much less time and with much less regulatory review. This gave him unprecedented authority with upper management which considered Tong to be *the expert* who could guarantee this to the Atomic Energy Commission (AEC). The managers themselves did not fully understand the technical aspects of DNB. Tong would make proposals to them to perform experiments which would allow an increase in the predicted CHF and which would in turn increase the power for their PWRs. Tong held this power over the managers so that he could not really be touched. Charlie didn't understand this scenario at the time.

Charlie and his group developed and modified computer codes such as SATAN-V for large pipe breaks and SLAP for small pipe breaks [4] which Westinghouse was using for licensing their PWRs. Before long Charlie realized that Tong understood two-phase thermo-hydraulic analysis of nuclear reactors only in terms of non-mechanistic correlations for the one-dimensional thermal–hydraulic model presented in his book [3] and did not adequately represent the physics of two-phase flow. The model assumed thermodynamic equilibrium and the single-phase homogeneous equilibrium mixture model (HEMM) with simplistic accounting of the relative motion between the liquid and vapor phases. There are important aspects of two-phase flow that just cannot be computed using such a model, such as steam–water countercurrent flow in the PWR downcomer and bubbles rising through stagnant liquid in the pressurizer. These phenomena were handled crudely using slip correlations and a bubble rise model, respectively [3, 4]. Charlie was convinced that this approach was inadequate and needed to be changed.

During his graduate education at IGT Charlie took courses in the Mechanical Engineering Department at IIT, he was especially influenced by the graduate course in continuum mechanics which he took from Professor Philip Hodge who used no text. He was taken by the idea that although a fluid's density is continuous down to a certain control volume size, it then begins to fluctuate wildly when molecular dimensions are encountered. Charlie was also influenced by teaching radiation heat transfer and numerical analysis in transport phenomena when he was an Adjunct

Assistant Professor with Dimitri at IGT between 1967 and 1968. Consequently, Charlie was able to formulate some ideas on how to develop a new theory of two-phase flow which would remedy the deficiencies in treating thermo-hydraulics as described in Tong's book.

But Charlie realized that he would never be able to pursue this under Tong's authoritarian rule and his progress was stifled. Tong would have daily meetings lasting one-half to 1 hour in length with each of his managers including Charlie to determine what advances each of their groups had made *the day before*. This was extremely stressful because analysis never proceeds that quickly. He also tried to force his solution technique on Charlie and members of his group to solve for perturbations of the equations as described on pages 211–212 in his book [3], rather than solving the equations directly using numerical techniques. This was a subject Tong knew little or nothing about and was the reason for which he had hired Charlie because of his expertise. So Charlie dismissed this technique as having extremely limited usefulness. When he found out that Charlie had not directed his group to proceed with the perturbation technique, he threatened to fire him and accused him of insubordination. Because of this intolerable situation, Charlie decided it was time to escape Tong's clutches and to leave Westinghouse.

Fortunately, Westinghouse itself provided an excellent opportunity on how to accomplish this escape. Dick Farman and Charlie were friends at Westinghouse. Dick was in an experimental group which was performing CHF experiments for the AEC at the Nuclear Reactor Testing Station (NRTS), now the Idaho National Laboratory (INL). This project was funded by the AEC at Westinghouse and managed by a good technical project engineer, Rex Shumway, at Idaho Nuclear Corporation (INC) which was replaced by Aerojet Nuclear Company (ANC) in 1971. Dick came to know the people at INC and was impressed with the outdoor activities in Idaho. He was anxious to go out west and was able to get a job offer in Larry Ybarrondo's Analytical Models Branch at INC. Charlie asked Farman for a contact so that he could apply for a job and wound up applying to Larry who offered him a position in December 1969. The recruiting company Charlie retained advised Westinghouse that he was looking for employment elsewhere. Tong approached Charlie and promised him that things would be different. Within a month, he was back to his usual browbeating. A manager parallel to Charlie, Jim Cermak, who had worked with Farman, told Charlie in confidence about a graph Tong had in his office where he plotted the pressure on Charlie daily. Sensing that Tong would not change, he kept Larry's job offer open.

So, in February 1970, Charlie decided to leave Westinghouse but not before he put in writing in his letter of resignation to Division management his reasons and heavily criticized Tong's management tactics. Charlie described in his letter how Tong was technically dishonest and had lied in the progress meetings describing his work. Charlie's Division Manager shared his letter with Tong, and this made him angry and vindictive. So, with that he left. Charlie was not the first to write such a letter criticizing Tong. We are quite sure that it was Duck Farman who had done so about two months before Charlie's resignation and left for Idaho. Little did Charlie suspect that Tong would recross his path again to orchestrate the destruction of one of the nation's finest scientific teams, the SLOOP Code effort to be described shortly in Chap. 5.

Larry Ybarrondo (Fig. 4.1) was kind enough to review my article [1] in the special issue of I&EC Research honoring Dimitri Gidaspow on his 75th birthday. Larry became the Manager of the Analytical Models Branch at INC. With his permission, I include edited excerpts of his narrative [5] which are germane to what the CFD and computer code situation was like at INC in the years before he hired Charlie Solbrig and before he started the SLOOP code project. It also touches on the loss-of-coolant accident and the RELAP series of codes.

Larry has, what he calls, a typical American background. He was born on July 15, 1937, in Detroit, Michigan. His mother was first-generation Irish/English. His father emigrated via a freighter bound for the USA from the Basque country of Northern Spain at the age of sixteen. When he arrived in Philadelphia, Pennsylvania, he swam from the ship to shore in the harbor with only the clothes he was wearing tied in a bundle on his head, with his belt under his chin. He spoke no English. He got a job on a railroad gang laying tracks. The Irish foreman made known to Larry's father that he needed to learn English and that the best place was the US Army. So, the Irish foreman took my father to an Army recruiting station having taught him to say, "I am eighteen" when asked how old he was. His father answered as instructed and served 4 years in the Army where he learned English.

After his military service, Larry's father moved to Detroit, where he met and married his mother. They had two boys and a girl. His brother died from a Korean

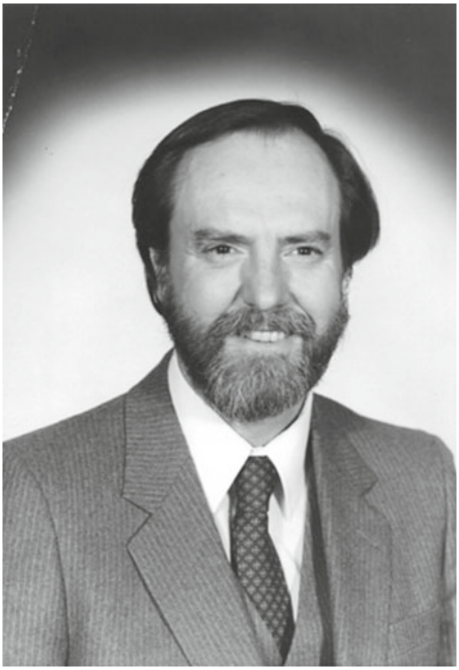

Fig. 4.1 Larry Ybarrondo at Aerojet Nuclear Company circa 1972 as I remember him

War wound. His education began in a Catholic elementary school, a Catholic high school, and the University of Detroit (a Jesuit University). He then enrolled in graduate school at Northwestern University in Evanston, Illinois, north of Chicago. He received a full Walter P. Murphy Scholarship, which included a tax-free $150 per month stipend. He graduated in 1962 with an M.S. in Mechanical Engineering. His M.S. thesis involving a thermoelectric device was patented and owned by Northwestern University. Larry then switched to Georgia Institute of Technology in Atlanta, Georgia where he received a Ph.D. in Mechanical Engineering in 1964. His Ph.D. dissertation "Thermoelectric Elements Utilizing Distributed Peltier Effect" was patented by Borg-Warner Corporation. Larry taught as an Assistant Professor of Mechanical Engineering at Georgia Tech for 4 years after graduating.

In June 1968, Larry moved to Idaho Falls, Idaho, to accept a position at the NRTS now known as the Idaho National Laboratory (INL). Initially, he was the supervisor of a group of four engineers tasked with developing computer codes for the AEC, independent of the commercial nuclear vendors. In order to fulfill its charter to assure public safety with respect to nuclear plants operations and potential accidents, it was essential to establish analytical and experimental capabilities to accurately predict and determine the nuclear, structural, chemical, radiological, thermal, and hydraulic transient phenomena present during a sudden complete offset sheer in a large primary system pipe and/or other postulated accident scenarios in any of the three commercial pressurized water reactor designs being built in the USA and abroad. Larry was instrumental in developing a power-to-volume scaling concept to generate meaningful experimental information which to assess the safety of commercial nuclear reactors. He was then assigned the responsibility for developing scaled experiments to assist the AEC to verify the analytical and experimental information being submitted to the AEC. Larry, his wife, and his sister currently live in California.

4.1 The "Loss-of-Coolant Accident" and the RELAP Series of Codes

What was the status of computer code development in July 1967? Engineers and physicists at NRTS were still using slide rules to calculate some of the input parameters for computer programs and to check calculations; think of pencils and paper. The first handheld calculators did not appear for several more years. The computer programs were typed on "IBM cards" at a "punch card" station. Then, the cards were put, in order of execution into a long rectangular box and submitted for running on the mainframe computer. The programs were generally run late at night, or very early in the morning, to get calculations completed because the US Nuclear Navy personnel had priority. It is easy to forget the primitive state of computer technology in 1967 through the mid-1970s compared to that of today. The computer at the NRTS in this time frame was an IBM 360/75 with a core storage memory of 130 KB and a magnetic drum storage of only 1 MB.

The analytical program to which Larry was assigned had four computer codes within its general area of responsibility: Some are described in "The 'Calculated' Loss-of-Coolant Accident–A Review" [4].

WHAM was a digital program used for the calculation of pressure, velocity, and force transients in liquid-filled piping networks and is an extension of the computer program **WATER-HAMMER** [6]. The model was used for predicting subcooled liquid-blowdown phenomena in support of an experimental section managed by George Brockett.

MOXY was used to describe two-dimensional core heat transfer phenomena using correlations from single-phase, steady-state flow data [4].

CONTEMPT The original author was Richard (Dick) Wagner. CONTEMPT was used for predicting pressure and temperature phenomena in pressurized water reactor containment during a 100% double-ended pipe break known as a large-break loss-of-coolant accident (LOCA). Small breaks were not yet considered in 1967 because it was assumed, erroneously, that the consequences of the 100% double-ended loss-of-coolant accident encompassed the consequences of the smaller pipe-break accidents. The code later became CONTEMPT LT [7].

RELAPSE-1 [8] was developed from the FLASH [9] code in 1966 at the NRTS and then run by the Phillips Petroleum Company. It was written in FORTRAN IV for the IBM-7040 and CDC-6600 computers. RELAPSE-1 was the nuclear primary systems analysis code to calculate the nuclear and thermal–hydraulic phenomena including pressures, temperatures, flow, mass inventories, reactivities, and power that occur during a postulated double-ended pipe break in which the ruptured primary system pipe ends were instantly offset 100% to allow maximum decompression of a PWR. This defines what is known as the loss-of-coolant accident (LOCA). These assumptions also maximized the structural forces generated during the single-phase subcooled liquid portion of the decompression. At a predesignated pressure after the pipe break, water from an ECCS was injected to keep the nuclear core from overheating.

Initially, the fluid flow equations used in the RELAPSE-1 code lacked critical terms. For example, the momentum flux term was missing. The three equations of mass, momentum, and energy were used to describe the steam and water being produced during the decompression. This is the HEMM model mentioned earlier. Basically, the equations and related empirical correlations were not sufficient to describe the transient, two-phase flow processes that would be occurring in a nuclear reactor during the transients of interest. At best, they were approximations. The steam bubble rise time value was input to the code by the user for the conditions being studied since it was difficult to determine experimentally. Larry recalls a story told to him by the authors Ken Moore, Walt Rettig, and Dick Wagner. They were in a local bar after work having beers discussing the importance of the steam bubble rise time and how to determine a credible value for it. One of them looked at the bubbles rising in his beer glass and said, "let's time the bubble rise." It was about three seconds. For a roughly 15-cm-high beer glass, this corresponds to roughly 5 cm/s. This value was subsequently used in calculations, and it worked, reasonably well, until more scientific data was available. Later a much larger value was recommended [4]. The state of the art in the late 1960s through much of the 1970s did not allow for a more complex set of two-phase flow equations. Why?

The computer codes of the late 1960s and early 1970s were in a very primitive state. RELAPSE-1 represented the primary system with just *three* lumped parameter control volumes (today they would be called mesh points or nodes) with pressure-dependent coolant pumps and a flow-dependent heat exchanger. The nuclear physics parameters, reactor coolant pump behavior, and safety system water injection were all done via input tables in the program. That is, there was no dynamic interaction between the core physics, heat transfer, fluid mechanics, and stored energy release into the fuel/cladding gap and thence to the cladding and fluid adjacent to the outside of the fuel rods. Fluid flow regimes were very difficult to impose and model, as were heat transfer coefficients, containment pressure versus reactor vessel pressure, and emergency core cooling injection. These items were all handled via predetermined input tables.

Interactive dynamic models were not feasible for many technical reasons such as available numerical techniques, applicable fluid regimes, heat transfer correlations, and computer performance capability, i.e., long computation times. The computer calculations also were very expensive, and so computer budgets were limited. For example, a single computer run with RELAPSE-1 might have taken on the order of 5 or more hours each depending on the parameters selected for analysis and cost on the order of $500/h. As Larry recalls, the annual computer budget for his analysis group by 1974 was on the order of ten to fourteen million dollars; a great deal of money indeed. The principal user of the NRTS Central Computer Facility was the US Naval Reactor Program which had priority use. Prior to about 1970 location of INC personnel with respect to this facility was an obstacle to effective communications because some of the engineers, mathematicians, programmers, and physicists doing the analytical work were located about 45 miles away from Idaho Falls at the Test Area North (TAN) site portion of the NRTS. Furthermore, the Central Computer Facility was located about 15 miles from TAN. Communications between these two sites were challenging because modern devices such as cell phones, laptop computers, and simple fax machines did not exist. One used a government car to get to where they needed to go and/or used the NRTS phone system which was not always dependable. At each facility, one needed to sign in/out and move through radiation detectors when entering and leaving. Portable radiation monitors were in place in a number of the facilities and sometimes alarmed. Communications were challenging! A major improvement was made when the Central Computer Facility and most of the engineers, physicists and support personnel were relocated to a single building in Idaho Falls in about 1969 which was the building in which I worked when I joined ANC in 1972.

The following questions arose that needed to be answered. What equations and first-order variables are essential to credible calculations that will withstand peer review? There was not an agreed-upon list of first-, second-, and third-order variables. See Rettig et al. [10], for example. This paper resulted from efforts to identify first-order variables in a disciplined manner. For example, what were the important effects and parameters associated with the LOCA in the PWR and BWR reactors and among the various configurations sold by each vendor? Ultimately, the Semiscale tests and rigorous analytical parametric studies were crucial in identifying the first-, second-, and third-order effect of the variables.

As the Semiscale (which simulated a nuclear reactor using an electrically heated core) experiments at NRTS progressed and more people used RELAPSE-1, it evolved into RELAP2, [11] RELAP3 [12] (both documented in reference [4]), and eventually RELAP4 [13]. The "RELAPSE" name was changed to "RELAP" along the way by Larry and accepted by the AEC, because it was really interested in progress rather than a "RELAPSE."

RELAP2 was released in 1968. It used the same three lumped parameter control volume representation of the system, the same leak/fill capability, and the same heat transfer model as RELAPSE-1 and incorporated models for boiling water reactors (BWRs). The program had improved stability and ran twice as fast as RELAPSE-1 on the INC IBM and CDC computers. In 1970, **RELAP3** evolved from RELAP2 and featured 20 control volumes, trip logic, valves, pressure-dependent fill and leak, fuel pins/plates, a heat conduction model and expanded heat transfer models. It was recognized that RELAP3 had serious deficiencies and work on RELAP4 was initiated to remove some of them. Work commenced, and in 1973, **RELAP4** was released. This code featured up to 100 control volumes, a momentum flux term, form losses, a two-fluid slip model, molecular nitrogen for the accumulator, representation of the secondary system as a flow network, and reflood heat transfer. The heat transfer capability was expanded to include modeling of reflood and a fuel gap. The zirconium–steam metal–water reaction was incorporated. A so-called implicit numerical method was introduced for time advancement to replace the former explicit time advancement [14]. This implicit method employs a linearized version of the field equations [15]. This implicit numerical scheme which was first incorporated into a version of RELAP3 replaced the forward difference, i.e., explicit time step advancement which resulted in extremely small time steps to maintain stability resulting in long computer run times. The result was up to an order of magnitude increase in time steps [16]. In addition to modeling small-break LOCAs for PWRs and BWRs, RELAP4 could also model large-break LOCAs. Solbrig and Barnum [17] present more details concerning the modeling capabilities of RELAP4. For schematics of the systems represented by RELAPSE-1 (same as RELAP2), RELAP3, and RELAP4, see Mesina [18].

At each stage of development, the codes were modified as experimental results were obtained and users in the USA as well as many foreign countries found various errors. A debate continued at INC on the equation set posed for use in these system analysis codes. The codes were frequently, to use a euphemism, "patched" as users from around the world used them on different BWR and PWR configurations, and therefore, conflicts developed internal to the code between the hundreds of subroutines. It got to be confusing to know exactly which version of the code a user was actually using.

So, a system called "Configuration Control" [19] was adopted to identify precisely which version and modification of the code a user was having difficulty with. It sounds simple in retrospect. But, keep in mind that this was about 40 years ago and coding practices were evolving rapidly. After a number of important modifications had been made, the code would go from being RELAP2, Mod X to RELAP2, Mod Y, etc. Eventually after major changes, the code name would be changed to RELAP3, Mod 1, and so forth. By the time RELAP4 was released, the code had been patched and modified so many times that it was clear and essential that what was needed was to start over with a "clean sheet of paper."

It was noted above that it was apparent to Larry and others when they joined his branch at INC that some terms were missing from the equation set being used in RELAPSE-1, RELAP2, and RELAP3. This was obvious to Larry because he had been teaching fluid mechanics, thermodynamics, and heat transfer courses for several years at Georgia Tech. They all agreed that some additional terms needed to be present in a properly posed set of fluid flow equations for normal, single-phase, transient fluid flow situations.

But the challenge in the LOCA situation was far more complex and challenging. Why? Briefly, during a LOCA, within milliseconds the highly subcooled water phase changes into a two-phase mixture of liquid and vapor. This mixture could be in the form of large slugs, small and larger droplets, and the vapor phase. These different forms of water/vapor could be traveling in the same directions at different velocities and/or opposite directions at different velocities. This was a huge technological challenge. As noted above, the state of computer memory capacity and speed, programming techniques, computer language capability, applicable numerical analysis methods, applicable and transient fluid and heat transfer correlations were not deemed to be adequate. So, yes, the momentum flux terms were missing from the fluid flow equations in RELAPSE-1, RELAP2, and RELAP3. The reason for the missing momentum flux terms had to do with some programming and numerical issues. The missing momentum flux terms were not the only technical issue that needed to be addressed.

4.2 A Mysterious Stranger Points the Way Forward

The following incident was revealed to me in Larry's document in which he reviewed my paper [5]. When Larry was the manager in charge of analysis development for INC in about mid-1969, he was informed by his immediate supervisor, George Brocket, that he was to meet a man in front of the DOE headquarters in Idaho Falls at 8:00 am the next morning. George did not know what the matter was about other than he had been informed that Larry was not to discuss his conversation with this man nor what would transpire subsequently with anyone—including George. Larry arrived at the appointed time and stood near the door. A man came up and introduced himself. A government vehicle was waiting at the curb with a driver inside. The man told Larry that he had been instructed to drive them both to the Naval Reactors Facility (NRF) building at the NRTS site. After they arrived, the driver left. They went inside where another gentleman met them and then took Larry to a small office area. As he recalls, this man did not introduce himself. The office had another door that was closed when they entered. The mystery man informed Larry that he had been selected to read a document and warned him not to discuss what he would read with anyone. He would have 1 h to read this document and could not have any paper or writing instruments to take notes. The man asked if he understood what he instructed and Larry simply replied "Yes." Larry was escorted into another room by opening the door which had been closed when they first arrived. It appeared to be a small conference room. In the center of the room were a single gray, government-issue table and chair.

Against the far wall was yet another man sitting in a gray government-issue chair. The man said to Larry, "Do you have any paper or writing instruments on you" to which he responded "No." The man then repeated what had been told to him by the man who brought him into the room, "You will have 1 hour to read the document on the table. You are not to discuss what you read with anyone. Is that understood" and Larry said "Yes." The first man left the room after which the seated man said, "You may begin." Larry sat down and looked at the document. It had labels stamped as he remembers, top and bottom "Top Secret" or "Secret." It was the computer manual describing the US Navy's classified version of the FLASH code. Even though he was stunned by this revelation, Larry began to read the table of contents carefully and tried to memorize the remainder of the document's contents as rapidly as possible in the hour allotted to him. When the end of that hour arrived the seated man said, "STOP" and Larry was ushered out of the room. As he left the man in the office reiterated to Larry not to discuss with anyone what he had read, nor his trip to the NRF building. To this he agreed and was taken back to Idaho Falls. No one including George Brockett ever mentioned this incident to Larry after it transpired and to this day he has no idea of the identity of the "Fairy God Mother" who arranged the trip and the review of the Navy's classified FLASH program document which confirmed to him that the INC RELAP computer code development program he headed was going in the right direction. He never discussed the matter with anyone until he revealed it to me. But, 30 years later, he thinks it is OK to tell this story. After all, no one was killed!

4.3 The Development of a Totally New Set of Two-Phase Equations

In Larry's recollection, Charlie Solbrig was the individual that pushed for immediate action on a proper equation set as soon as he was hired by him. And that he identified the need for two sets of equations for mass, momentum (analogous, to the single-phase Navier-Stokes equations), and energy: one set for the liquid phase and one set for the steam phase each of which could be traveling at different velocities and temperatures. Larry recognized that Charlie's thinking and approach were way ahead of the technology being used or even capable of being used at INC to analyze the LOCA properly. None of the nuclear vendors or foreign engineers that eventually participated in the loss-of-coolant test (LOFT) program had developed such a set of equations. Unfortunately, major obstacles remained. One was that the computer and numerical analysis technology available was not yet ready to be able to process the equation set Charlie was proposing. Also, there were technical peers in the industry and AEC that were not yet convinced of the need for the more complete equation set. Reasonable and knowledgeable technically trained professionals can disagree on the methodologies needed to resolve a technical challenge. Such was the case in this matter. As in many technical issues, one needed to be patient and resolve the problems one step at a time. That is what was done. For example, in the area of the numerical analysis methods used, there was a continual struggle to get, find, and develop numerical iteration techniques that would retain stability in the calculations. For example, the physical processes needed to be linked numerically and make sense physically. This did not always occur. Why?

For example, the occurrences of the critical physical processes varied from milliseconds to hours that would have made the numerical analysis techniques particularly challenging. Some promising conventional techniques, in such time intervals, did not function or resulted in illogical results such as “water packing,” more fluid coming into a nodal volume than was leaving with a decreasing pressure difference from the entrance to the exit of the node: This was physically impossible under the circumstances.

To summarize the preceding discussion, there were experimental data and phenomena that could not be described at all with the RELAP series of codes or FLASH and Charlie offered the way forward. However, it might prove to be an up-hill battle to convince management at INC and the AEC that a more complex approach would be the solution.

Charlie’s recollection on how the battle to pursue this new set of two-phase equations ensued complements Larry’s perspective. After Charlie went to work for Larry in February 1970, he found out from him that he was not that impressed with him or his ideas. Larry had four other managers working for him and Charlie was not yet a manager. Dan Hughes did not have any official connection with Charlie except his ideas appealed to him and he would bring articles on equations for multicomponent mixture theory. All of these articles only applied to a single-phase fluid. A good reference for this class of materials is the monograph by Drew and Passman [20]. None of these authors were trying to close the equations with correlations. None of them included imbedded stationary surfaces like fuel rods. Dan was doing Charlie a favor basically on his own time and so it can be said that Charlie developed the equations with encouragement from him. Charlie bounced all ideas off of Dan and then made corrections based on their discussions. Eventually Charlie produced a document incorporating all of his and Dan’s ideas [21]. The cover page and table of contents are reproduced in Fig. 4.2.

As the reader can see, all of the writing is in Charlie’s hand. He didn’t believe that he was in a strong enough position with Larry to have the manuscript typed by a secretary, and of course there were no word processors or personal computers available as yet. So, it stayed in the form of a manuscript. Much later this manuscript would be revised and published [22, 23].

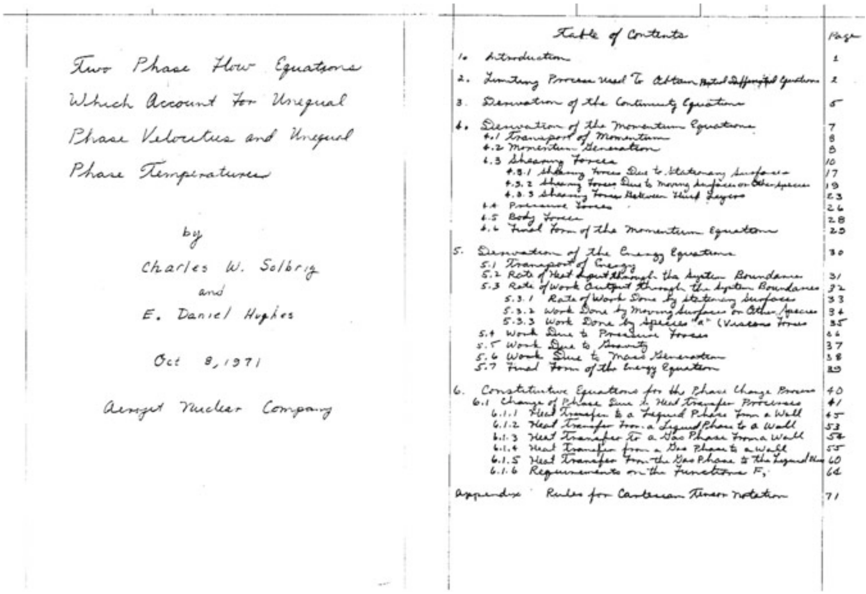

Fig. 4.2 Cover page and table of contents from the seminal handwritten document which was used to initiate the SLOOP code project at Idaho Nuclear Corporation for the AEC in 1971 [21]. The entire document can be viewed at https://www.osti.gov/scitech/biblio/1257862

Charlie had to continuously fight Larry's other managers who wanted to stay with the three volume RELAP2 representation of the PWR and thought that was enough detail. RELAP3 had not yet been released in early 1970 and initially could handle 20 control volumes [18] and later modifications or "mods" could handle up to 200 [4]. They thought Charlie was ridiculous. As mentioned earlier in this chapter, Charlie was significantly influenced by Philip Hodge, who taught his continuum mechanics graduate course at IIT and did not use a textbook. He said that the continuum representation for density was valid until one reduced the control volume size down to the size of molecules. Then it was necessary to take the limit as the control volume size approached zero assuming that the density was continuous and smooth. Charlie then realized that the same thing could be done for a two-phase flow down to the control volume size of bubbles or droplets and even larger for stratified or annular flow. Everything started to fall into place. Charlie called this new set of equations a "seriated continuum," that is, made up of a series of intertwined continua. This nomenclature has never really caught on. Some authors refer to the concept as interpenetrating continua [24]. He went off writing equations for each phase with imbedded stationary surfaces and heat sources. There was no precedent for this procedure, and so there were no guidelines as how to proceed—it was all done by intuition. The unique and unprecedented features of this document will be discussed further in Chap. 5.

So, the situation for Charlie early on at INC was the following. He was just hanging on by a thread doing what he was assigned to which was to convince people in charge of the various codes being used for analyzing the LOCA that they should be linked together. At the same time he was carving out time to work on the manuscript with Dan. Although Charlie had no one working for him, he was able to set up informal committees to get his ideas worked on, for example, the Idaho Nuclear Code Automation (INCA) paper [25] as well as putting together the monograph "The 'Calculated' Loss-of-Coolant Accident–A Review" [4]. The reason he could write this monograph was because Larry had him appointed as a consultant to the AEC's Advisory Committee on Reactor Safeguards (ACRS) and so he had access to General Electric's, Westinghouse's and Combustion Engineering's code manuals and safety analysis reports (SARs).

Dick Wagner who worked brilliantly on coding for the RELAP series of codes and Jay Larson, Dan's supervisor, were a real road block to new ideas. The committees muted them a bit. Charlie was eventually able to convince Larry and his boss George Brockett, Manager of the Nuclear Safety Development Branch, that RELAP3 should be replaced and he agreed to let him make a presentation to his sponsor Jerry Griffith at the AEC in Gaithersburg. In order to convince Jerry and other managers, Charlie would frequently use the PWR downcomer as and example where, during ECCS injection, water and steam flow countercurrent to each other—water flows down and steam goes up. The single-velocity nuclear reactor licensing code RELAP3 HEMM using bubble rise or slip models [17] was totally incapable of describing this situation. Charlie also argued that RELAP3, which treated the entire primary loop using three control volumes and the multivolume counterparts such as RELAP4 HEMM [18] could not represent with one velocity the phases which explosively moved in opposite directions. Charlie made view graphs of his handwritten report and would go through it page by page taking up to 3 hours to explain the equations and correlations to close the set in detail. Charlie relates that the AIChE monograph "The 'Calculated' Loss-of-Coolant Accident–A Review" [4] was pretty much what was in the so-called "White Paper" report which set off the heated inquiry into the adequacy of the ECCS analysis.

The Union of Concerned Scientists brought a legal suit against the AEC to stop the use of commercial nuclear power in the USA. They alleged such plants were not safe. Larry was one of about seven witnesses selected to testify concerning the status of commercial nuclear safety in the USA. He was sworn in by a Federal Judge in Bethesda, MD. Larry and several other engineers were grilled for several full days by corporate lawyers from the four nuclear vendors, Westinghouse, Combustion Engineering, Babcock and Wilcox and General Electric, assisted by top scientists, engineers, and physicists opposing nuclear power. Larry's testimony at those hearings is accessible in the government record system. I won't go any further into this part of the prehistory of the program since it is summarized in Carl Hocevar's monograph [26] and in Herbert Kouts' colorful speech given in 1998 [27]. It beautifully and succinctly summarizes the AEC/NRC history of nuclear safety research and the ECCS controversy. Since I don't think its existence is well known, I include it in Appendix B. Thomas Wellock, the official historian for the

NRC, has recently reviewed the ECCS controversy which included interviews with Larry Ybarrondo [28]. Suffice it to say, there was a great deal of controversy concerning nuclear reactor licensing involving the LOCA and the ECCS of which I was never quite aware of and in which I never became involved. Jerry bought the idea and initiated funding. Charlie got authority to have Dan work for him and shortly thereafter hired several programmers who were already at INC, e.g., Charles Noble, Robert Narum, or Carl Hocevar.

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Chapter 5
Project Development Begins

Nomenclature

Roman Letters

g	Gravitational acceleration
K	Drag function
P	Pressure
U	Internal energy
u	Velocity in x direction
t	Time
x	Coordinate direction

Greek Letters

α	Volume fraction
ρ	Microscopic material density

Subscripts

i	Phase i = solid or liquid
j	Phase j = gas or vapor

Let's back up a little now to the end of Chap. 3 and fill in what was happening to me before I finished up my doctoral dissertation and graduated from IIT in January 1970. The job market in 1969 was not very promising to put it mildly. There was a recession looming in early 1969. According to the National Bureau of Economic Research, the recession which was relatively mild lasted for eleven months. It began in December 1969 and ended in November 1970. This followed an economic slump which began in 1968 and by the end of 1969 had become serious. Industrial representatives visited IIT in early 1969 to interview students hoping to obtain

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employment after graduation. There weren't very many representatives, and none of them interested me. But for some obscure reason, I was attracted to the table where a gentleman representing Goodyear Atomic Corporation was sitting. He didn't look very busy (perhaps students were ignoring or avoiding him) and so I sat down gave him my resume and he began the interview. It turned out Goodyear Atomic was looking for a Gas Engineer!

Goodyear Atomic ran the Portsmouth Area Gaseous Diffusion Facility in central Ohio. This is where the isotope uranium-235 is enriched from its naturally occurring concentration and is subsequently used in nuclear reactor cores and atomic bombs. I told him I had a master's degree in Gas Engineering, was in the process of finishing my thesis for my Ph.D. in Gas Technology, and was planning to graduate in June. I also told him I obtained my undergraduate degree from Fenn College in Cleveland and so was familiar with northern and central Ohio. I got the feeling the representative was impressed with my credentials. However, I really don't think he had any idea what Gas Technology education at IIT was really all about. At any rate, I felt that the interview went quite well.

Shortly thereafter, I received an invitation to interview Goodyear Atomic on March 17. I was to fly to Columbus, Ohio. Arrangements were made for me to stay overnight on March 16 at the Holiday Inn in Chillicothe and then travel by rental car the next day to the plant site in Piketon for the interview. I don't remember much about the interview, but was impressed by the enormous magnitude of the buildings where the uranium hexafluoride in gaseous form was being enriched. I couldn't visit the enrichment facility itself, whose construction was begun in 1952, because that required a AEC "Q" level secret clearance. Piketon is pretty much in the middle of nowhere. The nearest cities of any size are Portsmouth, 20 miles further south on the Ohio River and Chillicothe, about 25 miles to the north where Meade Paper has a manufacturing plant. Upon returning to IIT, I wrote a letter to the person in charge of Employment Services at Goodyear Atomic thanking him for the interview and sent two reports on what I was working on requesting that they be forwarded to Dr. Woltz, one of only two Ph.D.'s at the facility and whom I must have interviewed.

On May 8, I received a letter from Mr. Prickett at Goodyear Atomic offering me a position in the Operations Analysis Department. The offer was contingent on passing their physical requirements, a satisfactory check of references (two of which were Charlie who was at Westinghouse and Dimitri), obtaining a security clearance "…within a reasonable length of time…," and completing my Ph.D. which I must have told them I estimated would be in August. I wrote a letter accepting the offer and then filled out the AEC Personnel Security Questionnaire along with fingerprints (taken for the first time!) in June. I must have hedged my exact date for starting employment in my letter of acceptance because, in a letter of July 1 from Mr. Prickett acknowledging its receipt, he expected me to join sometime in the fall.

As things turned out, putting all the loose ends together for my thesis took longer than I anticipated. Consequently, I informed Mr. Prickett that I would not be able to begin employment until November 30. I was getting worried that the offer would be withdrawn and I had not found any other job leads. Dan Hughes was experiencing the same kind of situation when he was finishing his doctoral dissertation in late 1968, through early 1969, when he was given a job offer by Larry Ybarrondo at INC. Well it looked likely that even that the start date of November 30 would slip, and so in my letter of November 15, I wrote that I anticipated a start date of the first week of January 1970 and pleaded to extend it. To my relief, a letter arrived on November 21 stating that this was acceptable and that a start date of January 5 would be acceptable. I finished up by the end of December, rented a small van and collected all my worldly possessions into it, and drove to Chillicothe. I reported for work on January 5, 1970. My AEC clearance had been completed and was given my badge and the title of Senior Engineer in the Operations Analysis Department. For a while I stayed in a hotel in Chillicothe and began searching for housing accommodations. Since I didn't have a car, I used the van for a short period of time. I vowed that I wanted to fulfill my dream of owning a Corvette, so I went to the Chevrolet dealer in Chillicothe and told the salesman to order one. For some reason, it was hard to find one, but shortly one was found with a powerful engine. I bought it and used it to commute to work. My first housing was in a rundown backwoods cabin in Piketon which looked like it had been vacant for a very long time. I stayed there a few weeks and then moved to nearby Waverly.

So I started in a part of the nuclear industry in January 1970, and Charlie joined INC in Idaho in February 1970 after leaving Westinghouse. He might have flown over Goodyear Atomic on his way there! And Dan Hughes was already at INC starting in early 1969. Some sort of destiny was in operation.

The work environment at Goodyear Atomic was, to put it mildly, not what I would have expected. I was shown to my desk in this enormous room where the desks and safes having combination locks to house secret documents of the total of roughly two dozen Operations Department engineers were located. There were no partitions—shades of the "bull pen" at Arthur G. McKee and Co.! I was assigned as a group leader of one maybe two other engineers. Next to this room was another room separated by a partition where plant operations engineers were located, also with no partitions between them. Across the hall were the offices of my supervisor Penrose Mellinge and his manager Dr. Woltz. The two-story building which housed most of the employees and upper management was a wooden, clapboard-sided structure probably erected in the early 1950s when the plant was constructed. It resembled an army barracks building. There was a computer which had stored in it the "inventory program." Acolytes would prepare computer cards from pressure drop data obtained in the gaseous diffusion cascade and submit them to the computer operator. The result was the total cascade inventory for the month. No one knew what the program in the computer was and it could not be changed. Sometimes there was a calculated "loss" of inventory from one month to the next which would mysteriously show up the next month. I was curious what the inventory program was and spent many hours in the library to determine its basis.

This also afforded me an opportunity to leave the bull pen environment where my desk and file safe were located. There I found many documents concerning the theory of the gaseous diffusion operation from the other plant at Oak Ridge, Tennessee. There were also quite a few documents in the secret part of the library authored by Klaus Fuchs, the spy who passed the secrets of the atom bomb to the Soviets! I started to put the pieces together into a document classified as secret. There was an ancient disused analog computer in the chemistry building where the library was located, about a mile away. I wasted quite a bit of time trying to program this beast, but gave up since no one could help me. At quitting time, all the engineers would line up and when this bell went off, they all ran out of the building to leave for the day. The first time this occurred, I couldn't believe it! I had no real assignment, but tidbits would occasionally be thrown my way. One of the more interesting ones was reviewing alternative processes to separate uranium isotopes such as shock waves in the Becker nozzle and acoustic mass separation. This was done in cooperation with a gentleman in the chemistry building who was assigned to this project with me. We would spend many relatively enjoyable days engaged in this project. I was given permission to attend a couple of AIChE meetings including one which I clearly remember, the 64th Annual Meeting in San Francisco, November 28–December 2, 1971. I was allowed to write a paper extending my master's thesis which was published in the AIChE Journal [1]. In 1972, I wrote up a report version of the fuel cell patent application submitted in 1969 (granted in 1974 [2]) with Dimitri and Bernie Baker which was used to satisfy the requirements to obtain my Professional Engineers License in Ohio. In spite of these few glimmers of professionalism, I soon decided I had to get out of this depressing job, but nothing was forthcoming.

After living for about half a year in a two-story rental house in Waverly, I decided to move. The house was flimsily constructed and had probably been built in the early 1950s during the construction of the gaseous diffusion facility. Most of the surrounding houses were of a similar construction. The owner of the one I rented owned several of them. When the wind blew, the house swayed slightly. Thanks to a referral, I found an amazing apartment in Chillicothe which was the former slave quarters of a huge mansion where the pastor of a local church lived with his family. It was accessible via a steep winding road to the top of a high hill upwind from the smelly Mead Paper Company. These structures must have been built in the early 1800s when Chillicothe was the first capital of Ohio. The walls of the renovated slave quarters were made of stone blocks about two feet thick and the ceiling of this two-story apartment was hewn from solid wooden dark walnut planks and beams. I struck up friends with Jack Woods, one of the employees, in the Operations Analysis Department who lived with his wife and two children a short distance from my apartment. He would drive his wife and myself to attend concerts of the Columbus Symphony. His wife, Nilufer, who was Turkish, worked as a chemist at the Mead Paper Company and was quite cultured and charming. Two years pass by in a blur.

5.1 I Am Hired by Charlie Solbrig to Work on the SLOOP (Seriated Loop) Code at Aerojet Nuclear Company (ANC)

As I was wasting away at Goodyear Atomic in Ohio, Charlie was busily putting his program together in Idaho after procuring funding from the AEC late in 1971 or early in 1972. A couple of important episodes occurred which would alter the course of multiphase science. This was Charlie's trips to visit Francis H. Harlow at what was then the Los Alamos Scientific Laboratory (LASL) later renamed Los Alamos National Laboratory (LANL). Charlie cannot recall the exact dates, but he is sure that there was one when he was at Westinghouse which would be before February of 1970 when Harlow was group leader of Group T-3, and another after he finished his handwritten report [3] and before I started at ANC on March 20, 1972. During his first trip, C. W. Hirt a member of Group T-3 (known to all as Tony) may have been present. He would leave LASL in late 1971 or early 1972 when he went to Science Applications Incorporated (SAI) for about two years and couldn't have been present at the second meeting. Tony returned to LANL in 1973 to replace Harlow as Group Leader. For his first meeting, Charlie says he went because he wanted to get advice on how to solve the equations which were germinating in his mind. Dimitri related to me that Charlie told him he went to see Harlow in order to "learn the ICE method." ICE, an acronym for implicit continuous-fluid Eulerian, was developed at LASL in the late 1960s to circumvent the Courant stability limitation for numerical solution of the single-phase Navier–Stokes equations [4]. This is more accurately referred to as the Courant–Friedrichs–Lewy condition, $(C\Delta t)/\Delta x < 1$, where C is the speed of sound, Δt is the time step size, and Δx is the mesh interval or size [5]. It's logical Charlie should visit Harlow at LASL since as Johnson demonstrates in his paper [4], the Fluid Dynamics Group T-3's achievements in CFD methods are legendary starting in the 1950s and extending through the 1960s and 1970s when Harlow was its Group Leader.

In Harlow's book completed shortly before his death on July 1, 2016, subtitled "Memoirs of a Los Alamos Scientist" [6], he refers to his paper published in 2004 [7] which he must have written around the time he retired from LANL in September 2003 after 50 years of continuous employment. His objective was to recount the "…many types of problems…solved for the first time with the newly emerging sequence of numerical capabilities…principally on these with which the author has been directly involved" [7]. Chapter 5, Los Alamos National Laboratory in Harlow's book [6] is quite terse and not very informative on what he accomplished in his 50-year career at LANL. In fact, the book is mainly about his passion for Pueblo pottery as evidenced by its title, fossil collecting, and his avocation of painting. So his paper is really the closest thing one could call Harlow's memoirs.

Charlie definitely insists he showed Harlow and Tony Hirt his handwritten manuscript and went through it in some detail, an incident he himself was to later regret. Charlie's impression was that "Harlow didn't know beans about two-phase." I am now going to get ahead of myself chronologically in the discussion that now follows because I want to present my thesis that before Charlie visited Harlow, his Group T-3 had never been involved in modeling two-phase flow and that it was only because of his historical 1971–1972 visit that they initiated multiphase code development. In fact, it was Charlie who started the science of two-phase flow and not Harlow as some may have the impression because they published first. Charlie's project relative to LASL's Group T-3 was in its infancy. In order to "test the air," so to speak, the venue used for presentation of progress was conferences and publication in their proceedings. Such proceedings are relatively inaccessible, and therefore the information tends to get lost. Harlow and his colleagues had been publishing in the Journal of Computational Physics (JCP) for decades. This journal was founded by LASL's sister laboratory Lawrence Livermore Laboratory (LLL) now Lawrence Livermore National Laboratory (LLNL). The primary mission of these two laboratories is weapons research. Therefore, LASL enjoys a special relationship with JCP publishing declassified results from weapons research. I hope to convince the reader of their lack of understanding the fundamentals of multiphase flow, their failure to acknowledge criticism of their work by, and the work of Charlie's Idaho group (due in large part of the AEC and later the NRC feeding LASL results of their progress or lack of it), and their lack of complete honesty. All of this qualifies as the politics of science.

There was a lull of several years before Harlow's first attempts to present methods to solve multiphase equations. In his paper Harlow describes in section "7. Multi-field flows (1971)" the difficulties they encountered [7]. The "1971" date is significant—this might refer to Charlie's visit otherwise why "1971"? There aren't any references to any LASL publications in this area in his paper until 1974. In referring to his reference 62 he states "…that the only results that could be meaningful are those that occur at scales significantly larger than the average value of that spacing,…" (referring to interparticle spacing) "…so that the problem of ill-posed behavior did not trouble us very much" [8]. This paper has nothing to do with solving multiphase flow equations—it refers to the multiphase numerical technique described to handle two or more single-phase fluids (multifluids) which should not be confused with multiphase flow. There is no discussion of ill-posed equations in this paper, a subject to be covered in Chaps 6, 7, and 8 later in this book. The KACHINA code published in 1974 [9] describes the LASL numerical method for solving the multiphase equations described in Harlow's references 64 and 66 [10, 11]. There is no reference in his paper [7] to any influence of, or reference to, Charlie's Idaho group's work at ANC on the SLOOP code project.

I asked Wen Ho Lee, a good friend of mine and with whom I worked with when he was at ANC, to call Harlow to ask him if he remembered Charlie's visit in about 1971. The reason I did this is because Wen and Harlow were good friends. They worked in different groups when Wen was at LASL with offices in adjoining buildings. They would frequently spend time discussing technical issues. Harlow's response was that he remembered "Idaho people" including Charlie visiting in 1971. When Wen asked Harlow when the development began, he didn't recall exactly, but estimated 1972–1973. With respect to the KACHINA code, Wen is of the opinion that such a large code would take about three years to develop. So 1971 plus three years equals 1974.

Now I am going into some technical analysis. Charlie wrote his equations in an obscure form using tensor notation which makes it difficult for a non-expert to fathom them. I will present them in the one-dimensional form as used in the SLOOP code. The continuity and inviscid momentum equations without transient flow forces or sources or sinks [12] may be written as:

Continuity equations

$$\frac{\partial}{\partial t}(\alpha_i\rho_i) + \frac{\partial}{\partial x}(\alpha_i\rho_i u_i) = 0 \tag{5.1}$$

$$\frac{\partial}{\partial t}(\alpha_j\rho_j) + \frac{\partial}{\partial x}(\alpha_j\rho_j u_j) = 0 \tag{5.1a}$$

Momentum equations

$$\frac{\partial}{\partial t}(\alpha_i\rho_i u_i) + \frac{\partial}{\partial x}(\alpha_i\rho_i u_i u_i) + \alpha_i\frac{\partial P}{\partial x} - K(u_j - u_i) + \alpha_i\rho_i g = 0 \tag{5.2}$$

$$\frac{\partial}{\partial t}(\alpha_j\rho_j u_j) + \frac{\partial}{\partial x}(\alpha_j\rho_j u_j u_j) + \alpha_j\frac{\partial P}{\partial x} - K(u_i - u_\mathrm{j}) + \alpha_j\rho_\mathrm{j} g = 0 \tag{5.2a}$$

In Eqs. (5.1) and (5.2), *i* refers to the liquid phase and *j* refers to the gas or vapor phase. Gravity, g, is assumed to act in the y-direction. The volume fractions are constrained by

$$\alpha_i + \alpha_j = 1, \tag{5.3}$$

since there assumed to be only two coexisting phases. The drag function, *K*, is flow regime dependent [13]. In Charlie's 1971 handwritten report [3], the volume fraction is inside the derivative in the pressure term given for phase *i* as:

$$\frac{\partial}{\partial t}(\alpha_i\rho_i u_i) + \frac{\partial}{\partial x}(\alpha_i\rho_i u_i u_i) + \frac{\partial(\alpha_i P)}{\partial x} - K(u_j - u_i) + \alpha_i\rho_i g = 0 \tag{5.2b}$$

$$\frac{\partial}{\partial t}(\alpha_j\rho_j u_j) + \frac{\partial}{\partial x}(\alpha_j\rho_j u_j u_j) + \frac{\partial(\alpha_j P)}{\partial x} - K(u_i - u_\mathrm{j}) + \alpha_j\rho_\mathrm{j} g = 0 \tag{5.2c}$$

During the development of the SLOOP code, both forms of the momentum equations, Eqs. (5.2) and (5.2b), were considered and analyzed. This led to part of the controversy concerning ill-posedness of the one-dimensional equations as will be discussed in Chaps. 6, 7, and 8.

The representation of the energy equations is more involved. The one-dimensional form of the energy equations derived by Gidaspow [13] using elementary thermodynamics is given by:

Energy equations

$$\frac{\partial}{\partial t}(\alpha_i \rho_i U_i) + \frac{\partial}{\partial \mathrm{x}}(\alpha_i \rho_i u_i U_i) = -P\frac{\partial \alpha_i}{\partial t} - P\frac{\partial(\alpha_i u_i)}{\partial x} \tag{5.4}$$

$$\frac{\partial}{\partial t}(\alpha_j \rho_j U_j) + \frac{\partial}{\partial x}(\alpha_j \rho_j u_j U_j) = -P\frac{\partial \alpha_j}{\partial t} - P\frac{\partial(\alpha_j u_j)}{\partial x} \tag{5.4a}$$

The right-hand sides of Eqs. (5.4) and (5.4a) represent the pressure work terms. Gidaspow [13] states that the first term on the right-hand sides of Eqs. (5.4) and (5.4a) involving the time derivative of volume fraction appears strange, but must be present in order that the mixture entropy is not violated. This term is missing in the energy equations written in total energy form (internal plus kinetic) in Charlie's 1971 handwritten report [3] which he showed to Harlow in his second meeting with him. It is also missing in Harlow and Amsden's first 1975 paper [10]. The spatial derivative of the pressure work term for both phases has been assigned completely to the equation for the vapor phase! There is no physical explanation as to why this should be. The result is that the mixture entropy equation may be violated. The analysis is given in reference [14], pages 278–280. Revelation of this problem was transmitted by Dimitri to Harlow shortly after publication of his paper [10]. Harlow totally disagreed with Dimitri's conclusion. The likelihood LASL would make such a serious blunder in handling the pressure work term is troubling. They must have been influenced by Charlie's handwritten report. If one writes the total energy equations he derived there in the form of Eqs. (5.4) and (5.4a), the time derivative part of the pressure work term is also missing. Harlow must be credited for using the momentum equation with volume fraction outside the derivative as in Eqs. (5.2) and (5.2a). It was shown in an unpublished memo that with the volume fraction inside the derivative with the pressure, unrealistic results would result [15]. Analyses such as this were the reason the momentum equations in the SLOOP code development in the form of Eqs. (5.2) and (5.2a), rather than Eq. (5.2b), were used. In addition, the controversy about the handling of this term and the ill-posed nature of the momentum equations had been swirling about for years before they published their first 1975 paper. The story of this controversy will be explained in Chaps. 6, 7, and 8.

By the time they published their second 1975 paper [11], the work terms were changed with no other explanation as to why or what motivated the change. Eventually, the SLOOP code development changed the energy equations to the form of Eqs. (5.4) and (5.4a), upon Dimitri's strong recommendation. In the years before the 1974–1975 series of three Harlow and Amsden papers were published, I will show in subsequent chapters that the SLOOP code was performing meaningful calculations and performing much due diligence in its research and learning constructively from their incursions into the dark and precarious science of multiphase flow modeling. I personally have not seen any truly convincing calculations involving the KACHINA code which, by the way, was never released, such as comparison with data or analytical solutions. This might be due to a lack of confidence in the results or deficiencies in the computer program. If anyone in Charlie's group tried to publish the type of the so-called Examples of Test Calculations presented in the two 1975 Harlow and Amsden publications [10, 11], I seriously doubt that JCP would accept their manuscript. Indications of hidden problems with the KACHINA code surfaced in the LASL Quarterly Report for the last quarter of 1974 in which was discussed that difficulties were noted when it was applied to sodium boiling dynamics analysis for liquid metal fast breeder reactor (LMFBR) problems [16]. The first difficulty noted is not accurately describing vaporization and condensation when the phase change rates are fast, as which would occur during a blowdown, resulting in unnecessarily small time steps. The second problem noted involved convergence problems during abrupt switching of the threshold volume fraction used during the iteration cycle.

So, what I hope I have demonstrated in the preceding discussion to the reader is that (1) Charlie's manuscript introduced LASL to multiphase modeling, (2) LASL showed a lack of understanding multiphase flow modeling, and (3) LASL never admitted to copying equations developed by Charlie's Idaho SLOOP code development group which resulted in their being less than completely honest.

What happened next must qualify as my third predestination event. Charlie called me in October or November, 1971, and told me that he had developed this new set of equations for two-phase flow and heat transfer, which he said were the equivalent to Bird Stewart and Lightfoot's [17] equations for single phase. He wanted to know if I was interested in joining in the program he was initiating. Without hesitation, I said I definitely would even though I was not quite clear what the job entailed since, as I have already described, was languishing at the gaseous diffusion facility in Piketon. In early November, I received an official application for employment and immediately sent it back in. I talked to Dimitri about the opportunity, and I will never forget what he said, "Charlie was modeling breaking pipes." This was Dimitri's inimitable way of boiling down a complex situation in his mind down to its essence. I thought this was quite a strange thing to be doing professionally and tried to picture the situation. Was this a mechanical problem or what? It didn't bother me since I trusted Charlie implicitly. In late December in response to my conversation with Morris Hillyard, ANC's employment representative, I was invited for an interview on January 10, 1972. Charlie who was in the System Model Development Section was to pick me up at 8 AM at the Westbank Motel where I was to stay from January 8th through the 10th. There was no need to be interviewed by Charlie so we chatted for the better part of an hour since we had not met since he left IGT in late 1968 when I was laboring on my doctoral thesis under Dimitri's guidance. The morning session of the interview started at 9 AM in the Central Computer Facility Building starting with E. Dan Hughes (who went just by "Dan") followed by Carl J. Hocevar, Glen A. Mortensen, and Robert (Bob) Narum, members of the System Model Development Section, then H. Donald (Don) Curet who was in the System Analysis Applications Branch, and finally William A. (Bill) Yuill who was the Leader of the Correlation Development and Material Modeling Section. After lunch I was interviewed by Larry J. Ybarrondo, Leader of the System Model Development Section and Charlie's boss, and George

Brockett, Manager of the Nuclear Safety Development Branch. These titles and assignments are what I pieced together from various ANC documents and memos. Aerojet Nuclear Company (ANC), whose parent Company was the California-based Aerojet General Corporation, had just taken over the Water Reactor Safety Program for the AEC from Idaho Nuclear Corporation (INC) on July 1, 1971, at the start of the NRTS fiscal year (FY) 1972. The Loss-of-Coolant Accident Analysis Program managed by George Brockett was a part of the Water Reactor Safety Program. Charles M. Rice, who was called "Chuck" by just about everyone and whom I did not interview, was General Manager of INC later to become General Manager of ANC. This transition was so recent that some forms used by ANC were left over from INC.

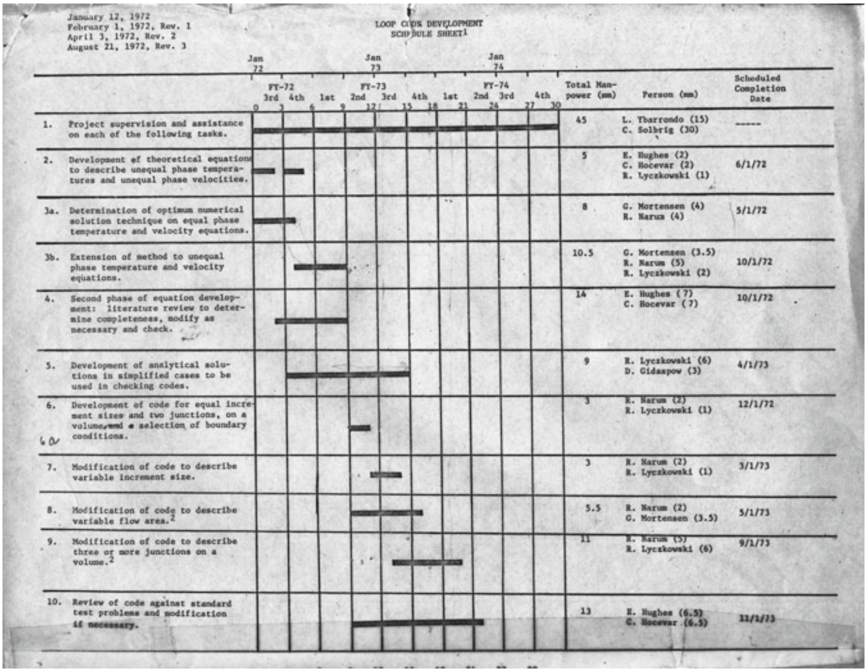
On January 31, I received a job offer by mail. It was as an Associate Scientist in the Nuclear Safety Development Branch with a salary of $1600 per month which I promptly accepted. The offer was contingent upon satisfactory pre-employment reference checks and qualification under AEC standards. This required me to fill out the lengthy AEC Personnel Security Questionnaire. I used a copy of the one I filled out to obtain my "Q" clearance for Goodyear Atomic to guide me, filled it out by February 6, and mailed it to ANC. I listed Charlie, Dimitri, and Frank Kulacki as references. There were several other contingencies attached to the employment offer including passing ANC's physical examination, ability to provide proof of birth, and ability to report to work as scheduled. In the letter of acceptance I indicated the week of March 19 or earlier. ANC arranged for an Idaho Falls moving company to pack and ship my household goods and personal effects. The packing was to occur on March 16 and shipped on March 17. ANC also arranged reservations for me to fly to Idaho Falls on Saturday March 18 and stay at the Westbank Motel beginning that evening. Just before I left Chillicothe and the moving company was soon to arrive to load my earthly belongings *and my Corvette* to move to Idaho, I received a letter in the mail dated March 15 from the State of Ohio State Board of Registration for Professional Engineers and Surveyors informing me that the qualifications for final professional registration were approved. What this meant was that the report based on the fuel cell patent application with Dimitri and Bernie Baker which I submitted to the Board earlier in the year (which was subsequently granted in 1974) [2] was deemed sufficient qualification for me to be registered as a Professional Engineer in the state of Ohio. With my departure from Chillicothe, I was freed from the possibility of a lifetime of meaningless drudge work at Goodyear Atomic, hurrah!

I joined ANC on Monday, March 20, 1972. My office was in the Computer Science Center (CSC), located near the western edge of Idaho Falls across from the Snake River near the airport, where the ANC mainframe computer, an IBM 360/75, offices for the CSC personnel, and those working on computer code development for the LOOP code, RELAP3, and other codes were located. To get to work Charlie would pick me up and drive me to the CSC. The ANC Headquarters, Idaho Operations Office, and AEC Headquarters were located downtown. When I joined, the other members assigned to work for Charlie's group included Dan Hughes, Carl Hocevar, Bob Narum, Glen Mortensen, Bill Yuill, Dick Farman, Kent Richert, and Bill Suitt from the CSC for computer support services.

I stayed in the Westbank Motel while I did some house hunting. I resolved to purchase a house with the savings I had accumulated working for Goodyear Atomic. Don Curet moonlighted as a real estate agent and started to show me houses for sale when he visited me at the motel. I wound up buying a nice home at 1439 Fairmont Drive located in the eastern part of Idaho Falls situated near a small shopping center. Carol Solbrig operated a gift shop in another larger shopping center near the central part of the city. I couldn't quite swing the down payment for the house I wanted, so I took out a small loan from a local Savings and Loan using some stock I bought in Chillicothe as collateral. When the moving van arrived in about a week, my Corvette and my worldly possessions were unloaded, were moved into the house, the boxes unpacked and distributed to the places I specified. My Corvette then became my means of transportation. It made it across the country without a scratch.

The great adventure had begun. The first thing I did was to assiduously study Charlie's manuscript describing the new equations. I still have a copy of his handwritten manuscript in my possession which contains the derivation of these equations [3]. As mentioned earlier, this material was eventually published in revised forms years later [12, 18]. I scanned it for Charlie during the preparation of this book, and he had it installed in the Office of Scientific and Technical Information (OSTI). The link to this document is included in [3]. The unique features of these reports are eight energy storage processes, five heat transfer mechanisms, seven wall heat transfer regimes, seven interphase and wall friction forces, thirteen flow regimes, which formed a complete set of constitutive relations to close the equation set.

The thing that struck me was the incredible amount of planning that had gone into the LOOP Code Project (its name was not decided upon yet) in the two years since Charlie joined ANC in February, 1970. The first page of the August 21, 1972, revision of the LOOP Code Development Schedule Sheet is shown in Fig. 5.1. Manpower in man-months (mm) and personnel assigned for each of the tasks 1 through 10 are shown together with scheduled completion dates. It is quite clear revisions were proceeding at a brisk pace early on as indicated in the top left. There are a total of 30 tasks! The planned time span for the LOOP code development was two and a half years from January 1, 1972, to June 30, 1974. In the first version of this schedule sheet dated January 12, 1972, I was penciled in as "New Hire #1". These schedule sheets would soon become the dreaded management by objectives (MBO) management system employed by ANC. Individual MBO schedules were later required for each person and signed by them. Figure 5.2 contains a flow chart indicating how the various tasks would flow as they progressed and were completed. From the Schedule 189a (a form used to justify obtaining funds from the AEC) for FY 1973 the total estimated manpower requirement listed for FY-1972 was sixteen man-years for scientific staff and five for support activities for a cost including overhead about twice salaries (mine was about $20,000/year) for a total of close to $1 million. That would be close to $10 million today. The man power and funding levels for FY-1973 and FY-1974 were projected to be about the same. What is clear is that the SLOOP code effort was not a two-person effort like the



January 12, 1972
February 1, 1972, Rev. 1
April 3, 1972, Rev. 2
August 21, 1972, Rev. 3

LOOP CODE DEVELOPMENT
SCHEDULE SHEET[1]

Jan 72 · Jan 73 · Jan 74

FY-72: 3rd 4th · FY-73: 1st 2nd 3rd 4th · FY-74: 1st 2nd 3rd 4th

0 3 6 9 12 15 18 21 24 27 30

		Total Man-power (mm)	Person (mm)	Scheduled Completion Date
1.	Project supervision and assistance on each of the following tasks.	45	L. Ybarrondo (15) C. Solbrig (30)	-----
2.	Development of theoretical equations to describe unequal phase temperatures and unequal phase velocities.	5	E. Hughes (2) C. Hocevar (2) R. Lyczkowski (1)	6/1/72
3a.	Determination of optimum numerical solution technique on equal phase temperature and velocity equations.	8	G. Mortensen (4) R. Narum (4)	5/1/72
3b.	Extension of method to unequal phase temperature and velocity equations.	10.5	G. Mortensen (3.5) R. Narum (5) R. Lyczkowski (2)	10/1/72
4.	Second phase of equation development: literature review to determine completeness, modify as necessary and check.	14	E. Hughes (7) C. Hocevar (7)	10/1/72
5.	Development of analytical solutions in simplified cases to be used in checking codes.	9	R. Lyczkowski (6) D. Gidaspow (3)	4/1/73
6.	Development of code for equal increment sizes and two junctions, on a volume, ~~and~~ a selection of boundary conditions. 6a	3	R. Narum (2) R. Lyczkowski (1)	12/1/72
7.	Modification of code to describe variable increment size.	3	R. Narum (2) R. Lyczkowski (1)	3/1/73
8.	Modification of code to describe variable flow area.[2]	5.5	R. Narum (2) G. Mortensen (3.5)	5/1/73
9.	Modification of code to describe three or more junctions on a volume.[2]	11	R. Narum (5) R. Lyczkowski (6)	9/1/73
10.	Review of code against standard test problems and modification if necessary.	13	E. Hughes (6.5) C. Hocevar (6.5)	11/1/73

Fig. 5.1 First page of the LOOP Code Development Schedule Sheet revision 3 for the period January 1, 1972, to June 50, 1974

KACHINA code where there was one theoretician (Harlow) and one programmer (Amsden). In the LOOP Code Project, there was an abundance of each. This engendered interaction and feedback among the team members. As time went on, each contributor would issue internal memos documenting progress and problems encountered. There was no hiding sloppy work!

Perhaps because of the recent transfer of the Water Reactor Safety Program for the AEC from Idaho Nuclear Corporation (INC) to ANC just six months previously, and the new monies rolling in for the LOOP Code Project, there were reorganizations afoot. Just days after I joined ANC, General Manager Chuck Rice issued a Management Bulletin explaining the situation whereby groups were being consolidated, why it wasn't possible to hire people to do some jobs, why functions were being eliminated, why people were being transferred to different divisions, and why a few people were being terminated. The reason given by Rice was that resources had to be applied to high-priority work while curtailing lower-priority programs. On May 15, 1972, Charles K. Leeper was appointed as President and General Manager of ANC replacing Chuck Rice. On December 5, 1972, Larry Ybarrondo was appointed Branch Manager of the Analytical Development Branch

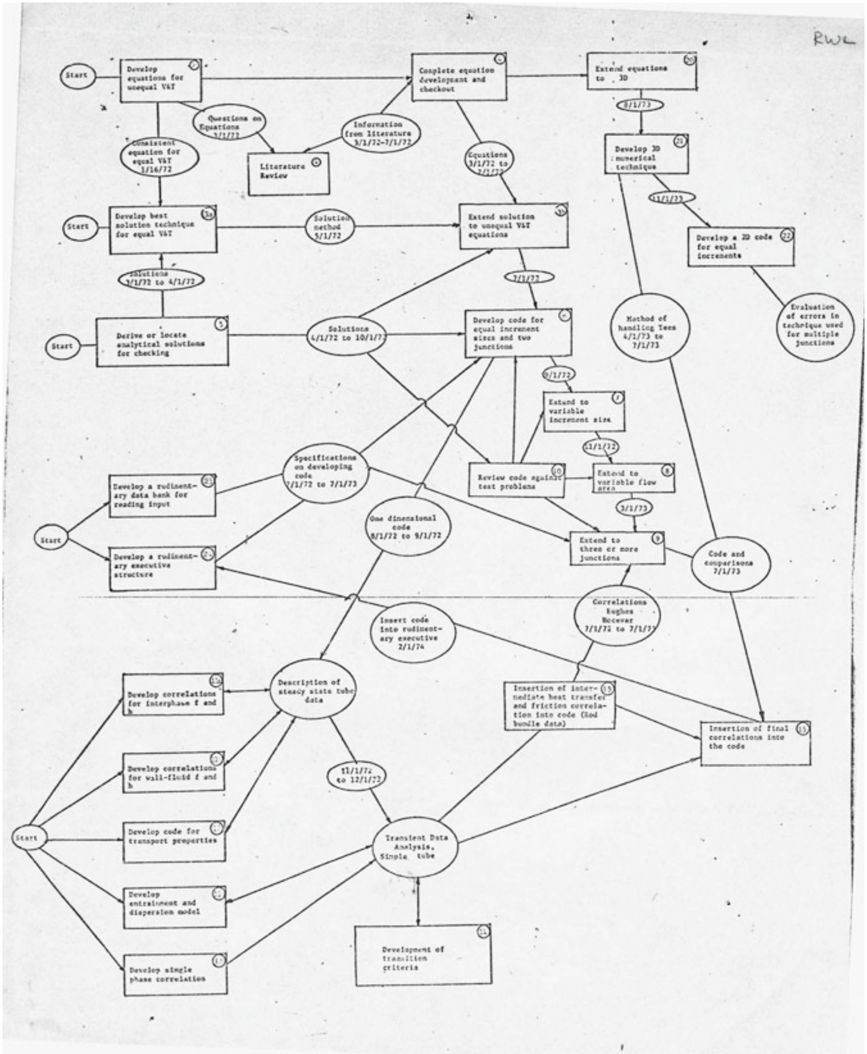


Fig. 5.2 Flow chart indicating the relationship between the various LOOP code tasks and their completion dates

and Charlie replaced him as Leader of the System Model Development Section. It appears that at about the same time the Water Reactor Safety Program Division was renamed the Thermal Reactor Safety Program (TRSP) Division and George Brockett was demoted from Manager of the Nuclear Safety Development Branch to the TRSP planning staff. At the same time the charter for the TRSP and its five branches was announced. The charter for the Analytical Model Development Branch was defined as:

> Produce an integrated system of safety assessment analytical techniques which will adequately: (a) predict the course of abnormal behavior of large thermal reactors, and (b) determine the desired performance (sic) of engineered safety systems for postulated abnormal or accident conditions for a particular plant.

Just one month later on January 8, 1973, Larry was appointed Manager of the LOFT Program Division and Charlie became Manager of the Analytical Development Branch. On February 5, 1973, Peter M. Lang became Manager of the TRSP. What a dynamic organization was ANC. After this reshuffling of managers, things appeared to settle down.

I can only describe what I encountered as I got down to work that this was a ten-ring circus. Compared to the staid work environment at Goodyear Atomic, this was order of magnitude more stimulating and challenging. My brain cells switched into high gear and activated my imagination and creativity. I started contributing to the program in short order, issuing a constant stream of letter reports and interoffice correspondences documenting my findings and accomplishments. This was going to be quite an experience—it was like starting another Ph.D. or maybe two!

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Chapter 6
Characteristics Analysis of the One-Dimensional, Two-Fluid Partial Differential Equations (PDE's) Developed by Charlie Solbrig and Dan Hughes

Nomenclature

Roman Letters

A Matrix
B Matrix
C Speed of sound
g Gravitational acceleration
K Drag function
P Pressure
U Vector of dependent variables
u Velocity in x direction
t Time
x Coordinate direction

Greek Letters

α Volume fraction
λ Eigenvalue of the characteristic polynomial = dx/dt
ρ Microscopic material density

Subscripts

i Phase i = solid or liquid
j Phase jK = gas or vapor

Superscripts

T Transpose

What follows now is one of the central narratives in this book. It constitutes the description of one of the most traumatic and drawn-out series of events in the

R.W. Lyczkowski, *The History of Multiphase Science and Computational Fluid Dynamics*, Mechanical Engineering Series,
https://doi.org/10.1007/978-3-319-66502-3_6

SLOOP project's brief existence (and in my career): the issue of the complex characteristics of the two-phase basic equations. The first important narrative dealt with the politics of science involving the origin of these equations as recounted in Chap. 5. Another aspect of that story unfolded during the course of the SLOOP code's life span of just over three years. Beginning with this chapter and extending over the next two in Chaps. 7 and 8, there was such a torrent of events that it will be difficult to recall all of them accurately after the passage of over 40 years. I will attempt to present a roughly chronological order of events as well as the individuals involved in this narrative. Some events are pinpointed fairly exactly since they are documented in conference proceedings and in correspondences.

Dimitri went out to Idaho to consult for Charlie on his new project in early 1972 before I joined ANC. He followed it up with his sabbatical from IGT in 1973 which will be discussed in Sect. 6.1. Dimitri still has his ANC badge which he displays proudly in his office in Perlstein Hall at IIT. I scanned it, and it is shown in Fig. 6.1. In a sense, I was literally following in his footsteps. He was to be the project's very first consultant. This would not be Dimitri's last consulting experience by any means. Later, as the project progressed, there would be more consultations as well

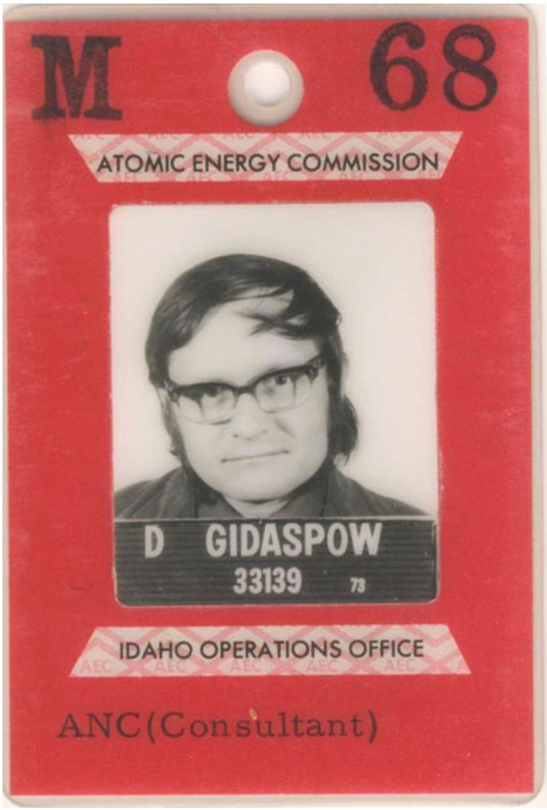

Fig. 6.1 Dimitri's ANC Badge, 1973

as additional consultants. Charlie had received no help from Frank Harlow from his visit to LASL. Dimitri had taught the course Numerical Methods In Transport Phenomena at IGT with some lectures given by Charlie. Thus Dimitri was the ideal candidate to seek for advice. I took this course which resonated with me significantly. I took careful notes which I consulted frequently in my subsequent career. Only decades later would Dimitri include them in his second book [1]. Charlie went over the concepts and equations with Dimitri using his handwritten report [2]. As I mentioned in the last chapter, I called Dimitri before I joined ANC to get his advice. He had a strongly positive recommendation for Charlie's project which I joined shortly after Dimitri's visit. Charlie had done all of this planning as evidenced by the LOOP code development schedule sheet and flow chart shown in Figs. 5.1 and 5.2. With Dimitri's positive feedback Charlie's project started in earnest and shortly thereafter things were off and running.

It must be pointed out that there were no courses in two-phase flow at IIT (nor any place else to my knowledge), so the equations were new to Dimitri. In fact they would be new to just about anybody looking at them. They looked vaguely familiar to the one-dimensional Navier–Stokes equations, one for each phase. However, there was a new variable floating around in them, the volume fraction of each phase. In his book published in 1969 Graham Wallis included the section that he called "One-Dimensional Separated Flow in Which the Phases are Considered Separately" [3]. There is no derivation for the momentum equations just the explanation "…The momentum equations, equations of motion, or Newton's law for the two phases can be written quite generally in three-dimensional vector form…". In fact, if the momentum Eqs. (5.2) and (5.2a) are written in non-conservation law form, they bear a strong resemblance to the single-phase momentum equations but with the addition of subscripts,

$$\rho_i \frac{\partial}{\partial t}(u_i) + \rho_i u_i \frac{\partial}{\partial x}(u_i) + \frac{\partial P}{\partial x} - f_i + \rho_i g = 0 \tag{6.1}$$

$$\rho_j \frac{\partial}{\partial t}(u_j) + \rho_j u_j \frac{\partial}{\partial x}(u_j) + \frac{\partial P}{\partial x} - f_j + \rho_j g = 0 \tag{6.2}$$

which are identical to Wallis's Eqs. (3.45) and (3.46) with his body forces b_i and b_j representing the gravity terms above and $f_i = K(u_j - u_i)/\alpha_i$ and $f_j = j = K(u_i - u_j)/\alpha_j$, which could be interpreted as Wallis' "what is left over" terms, f_i and f_j. He goes on to do some analysis using these equations. Wallis' book was not known to Charlie or Dimitri (or myself) at the time (1972), and even if it was, would have had no significant influence on the course of events which were about to unfold.

One of the things Dimitri highly recommended to Charlie was that the one-dimensional partial differential equations (PDE's), which were to be solved by programing them into the SLOOP code, should be analyzed using the Method of Characteristics (MOC) [4]. This is a necessary task because the nature of the equations, be they hyperbolic, elliptic or parabolic, determines their method of solution and how to apply appropriate boundary conditions. Wallis does not solve his equation numerically nor does he obtain the characteristics for them. Dimitri taught MOC in his course Numerical Methods in Transport Phenomena at IGT. As discussed in Chap. 4, the SLOOP code was to be a one-dimensional transient code to replace RELAP4 [5], the successor to RELAP3 [6], as discussed in Chap. 4 and might even have become RELAP5 whose origin is discussed in Chap. 10. Recall that these nuclear reactor licensing codes, like the ones used by the vendors, including General Electric, Westinghouse, Babcock and Wilcox, and Combustion Engineering, assumed equal phase velocities and temperatures, the homogeneous equilibrium mixture model (HEMM) [7]. These equations are hyperbolic and therefore can be solved as an initial-value problem. That is, initial conditions are prescribed at time zero and with appropriate boundary conditions, and the solution is obtained numerically by marching a finite difference set of equation forward in time.

With Dimitri back at IGT in Chicago to teach, I alone was ready to take up the gauntlet to determine the characteristics of Charlie's two-phase equations. At this stage, we were not aware of Wallis's momentum equations, so we using Eqs. (5.2b) and (5.2c). With nothing to guide me except my notes from Dimitri's course on numerical methods, I started by trying to determine the characteristics for Charlie's set of two-phase equations. These equations looked so simple to analyze, BUT and that is a BIG BUT, that would turn out not to be. Single-phase flow for say, water or gas, has only three equations. The characteristics are well known; they are the phase velocity and the phase velocity plus or minus the speed of sound.

There was so much going on simultaneously in Charlie's group that I decided to concentrate on the tasks assigned to me. At the beginning of the SLOOP code project, these tasks were broadly stated with a lot of leeway in their exact interpretation. Referring to Fig. 5.1, clearly Tasks 2, 3a and 5 allowed me the flexibility of trying to determine the nature of Charlie's equations using MOC. From here on out in the rest of this book, I am going to try to document key activities and events with which I was personally involved and upon occasion summarize others performed by the other member of the LOOP code. This won't be easy after the passage of over four decades, but I'll try.

I started my tasks for the first few months by writing out, as an exercise, a set of difference equations to solve Charlie's equations. The overarching ground rule was to use fully implicit central differences for spatial derivatives because this numerical method is unconditionally stable, at least for the diffusion equation [8]. Combination of the continuity and momentum difference equations is used to form a Poisson equation for the pressure, similar to that for the ICE methods developed by the LASL Group T-3 [9, 10]. Using the same rigor taught by Dimitri and Charlie in the IGT numerical methods course, I made sure that the number of unknowns, 14, was equal to the number of equations. I don't recall that this write up made much of an impression on the other members of the group, but at least I tried. Then I moved on the determining the characteristics for these equations.

To begin with I studied various techniques in the literature explaining how to obtain the characteristics. This included the MOC methods described by Abbott

[11], Von Mises [12], and Sedney [13] to, so to speak, gird my loins and guide me for the, as it turned out to be, formidable task of obtaining the characteristics for the set of six equations, two each for continuity, momentum, and energy. None of these three literature sources gave clear-cut examples on how to proceed so I forced myself through their methodologies using first as an example, the equations for the transmission of natural gas [14]. Each method took pages to get to the answer. This occupied me for the better part of 1972, and I had already stopped looking at the LOOP Code Development Schedule Sheet which I kept taped to the wall in my office. As I recall, nobody was helping me so I wrote up my findings as soon as I could cast them into what I considered a definitive, i.e., coherent form, and circulated them to others in the group. I don't recall much feedback.

Next I applied the Sedney MOC method to obtain the characteristics for the three single-phase HEMM equations which would be programmed into a code called EVET (Equal Velocity Equal Temperature) to evaluate numerical methods and boundary condition treatments. Lessons learned here would be useful when the full set of six SLOOP code UVUT (Unequal Velocity Unequal Temperature) equations were programmed and running. The acronyms EVET, UVUT, and later other combinations such as UVET, EVUT, and EVE, even ZVUT (where E stands for Equal and Z stands for Zero) turned out to be useful to quickly convey to members of the group which equations were being discussed. These acronyms eventually caught on with some researchers outside of our group and even with the AEC sponsor. I not only obtained the characteristics for the HEMM equations, I also obtained the compatibility conditions as well. This analysis would eventually be published as part of Section 4.5 in reference [15]. My remaining notes were never cleaned up nor published.

As time went on, it was possible to boil down the procedure to determine the characteristics to a simple procedure. First, the system of first order partial differential equations (FOPDE's) are written in the form:

$$\mathbf{A}\frac{\partial \mathbf{U}^T}{\partial t} + \mathbf{B}\frac{\partial \mathbf{U}^T}{\partial x} = 0 \tag{6.3}$$

A and **B** are matrices containing the terms multiplying the temporal and spatial derivatives, respectively, and $\mathbf{U}^T$ is the transpose of the column vector containing the dependent variables. Then the eigenvalues, i.e., the characteristic directions or simply what I have been calling the characteristics, λ, are determined from the characteristic polynomial resulting from,

$$\det(\mathrm{A}\lambda + \mathbf{B}) = 0 \tag{6.4}$$

where det stands for the determinant.

Now I was ready to tackle the problem of determining the characteristics for Eqs. (5.1), (5.1a), (5.2b), (5.2c), (5.4), and (5.4a). This was more easily said than done. At this time, we as well as I assumed that Charlie's momentum equations with the volume fraction inside the derivative with the pressure Eq. (5.2b) were correct. For what seemed like months, I struggled to find the characteristics for this case. Meanwhile, back in Chicago, Dimitri was also trying to analyze this set of equations. We were both stumbling in the dark. I used the MOC method of Sedney to obtain two characteristics as equal to the phase velocities given by $\lambda_1 = u_g$ and $\lambda_2 = u_l$. It was not clear at this early stage where they came from. Later we learned that they originated from the energy equations if they were correctly written in entropy form. See page 279 in reference [15]. The other four characteristics were tied up in a fourth-order polynomial that simply would not factor! I was able to arrange it into the following form,

$$\left[(\lambda + u_g)^2 - C_1\right]\left[(\lambda + u_l)^2 - C_2\right] = C_3 \tag{6.5}$$

where C_1, C_2, and C_3 are complicated functions of phase densities, speeds of sound, volume fractions; and pressure. For the limiting case of all liquid and all vapor, the characteristics reduced to the single-phase characteristics and the phase velocities. However, for the case of equal velocities, it was not clear that the characteristics were real or not. I tried valiantly to use the formula for finding the roots of a quartic equation [16]. The method requires reducing the quartic equation to a cubic equation and then using the method for finding its roots. Unfortunately, because of the enormous amount of algebra involved, I gave up.

6.1 Dimitri's Sabbatical and the Discovery of Ill-Posedness (Complex Characteristics) of the PDE's

The situation had become extremely frustrating for me since Charlie's equations, which looked so simple produced this messy impasse, not easily resolvable. Dimitri was stymied as well. The focus was now to evaluate, somehow, this forth order polynomial. This effort continued for all of 1972 and spilled over into early 1973. Dan Hughes and Glen Mortensen were drawn into the fray. Charlie's sporadic 1972 Monthly Management Reports for the System Model Development Section to Larry played down the characteristics impasse. In May 1972, it was reported that "A study was conducted to classify the basic equations." Progress by the rest of the group on tasks listed in the LOOP Code Development Schedule Sheet (Fig. 5.1) *was* reported. A notable example was Glen Mortensen's writing a program called STAB using the IBM FORMAC computer program which could, for example, evaluate determinants of matrices, multiply them, and invert them symbolically [17]. He used this program to automatically investigate the stability of the finite difference equations and numerical iteration schemes to solve the systems of PDE's for the HEMM equations which were being programmed into the EVET code for Task 3a (see Fig. 5.1). Even for the three PDE's and an equation of state, this is a mammoth task requiring the analysis of no less than 24 different iteration schemes to find those which are stable. In December 1972, it was reported that the EVET code was running but was having problems. Once again Glen's FORMAC program was used to track down a resolution. Stability of the difference and iteration schemes would turn out to be a recurring theme which slowed down progress on developing the SLOOP code. Progress was reported on the programming of a model for CHF and film boiling, Task 15, and the development of a rudimentary Executive code, Task 24a. Lack of progress or difficulties were not reported. Weasel words like "were developed", "work is continuing", and "improvements were made" were used. At first, these monthly reports were extremely informal, even to the point of containing handwritten material. I highly doubt that they got passed on to management above Larry. One reason for this might have been the frequent reorganizations discussed earlier in Chap. 5, Sect. 5.1. I briefly reiterate these organizational changes in order to demonstrate how quickly changes were being made around me. On December 5, 1972, Larry became Manager of the Analytical Models Branch and Charlie replaced him as Leader (at various times, the title was either Manager or Supervisor) of the System Model Development Section where I was situated. On January 8, 1973, Larry became Manager of the LOFT Program Division and Charlie became Manager of the Analytical Models Branch which was subsequently renamed the Analytical Model Development Branch. On February 8, 1973, Pete Lang became Manager of the TRSP. At this point, the monthly reporting procedure became much more formal. The February 1973 report for the System Model Development Section was now included in Charlie's Monthly Management Report of Analytical Model Development Branch which was then rolled into Pete Lang's Thermal Reactor Safety Program Monthly Report to the Director of the Idaho Operations Office of the AEC for patent clearance prior to issuance for outside distribution. Charlie appointed me as Section Leader, and I started being listed along with Bill Yuill as one of the authors of the System Model Development Section report. I was also signing the new, improved, and much more formalized versions of the LOCA Analysis Flowchart shown in Fig. 5.2 that now became ANC's program (or project) evaluation review technique, commonly abbreviated as PERT, network chart.

In discussions with Charlie, it was decided to give Dimitri a contract and to bring him back to Idaho Falls and to work with me to straighten out the classification impasse for Charlie's equations. Just after Charlie became Branch Manager, I was assigned to send an Interoffice Correspondence to George Brockett requesting him to procure Dimitri's contract. On January 11, 1973, I wrote this draft titled "Report Purchase from Professor Gidaspow". In it I tried to justify why this was necessary. Apparently, George had his assistant R.B. Benjamin, who previously had been charged by him to prepare the formal PERT for the Water Reactor Safety Program Division, suggested changes to this correspondence. My revised correspondence was revised and sent to George on January 22. It was further massaged by George but preserved the essence of what I wrote and sent to procurement on February 1. This letter is a classic and I quote some excerpts from it,

> The basic theoretical equations are essentially complete. Analytical solutions should be obtained for this equation set with certain simplifying assumptions such as incompressibility, isothermality or isotropy and decoupling at the phase boundary. Analytical solutions are used as quality control procedures for the numerical computations resulting from

> existing codes for relatively well understood test problems. Solutions can also be used to interpret unexpected phenomena, resulting from running other test problems on existing and future codes.
>
> We request to purchase a report from Professor Dimitri Gidaspow, Department of Gas Technology, Illinois Institute of Technology in the area of analysis and transport phenomena which present additional analytical solutions which we would use for quality control purposes. Application of compressible flow theory, method of characteristics, Green's functions and potential theory to obtain solutions would be required.

The seven page subcontract was drawn up and sent to Dimitri on February 14 to sign which he did on February 27, 1973, witnessed by Darsh Wasan who was (and still is) in the Chemical Engineering (now Chemical and Biological Engineering) Department at IIT. The work was to run from February 15 to August 31, 1973. The Appendix to the subcontract boiled down the Scope of Work to "Generate a set of analytical solutions which will be used as quality control procedures for the numerical computations relating to the LOOP code. This will include simplifying assumptions such as incompressibility, isothermality and isotropy and decoupling at the phase boundary." There is no mention of a report required. In addition to Dimitri's fee for his time consulting, he was to be reimbursed for two round trips between Chicago and Idaho Falls. I call upon the reader to imagine what a contract like this would look like if ANC paid Albert Einstein to write a report to develop the equations for Special and General relativity.

Dimitri flew out to ANC in March 1973 to begin his sabbatical right after his subcontract was in place. He was issued his new picture badge shown in Fig. 6.1. When he was in Idaho Falls he stayed at the Westbank Motel. One of his priorities was that he wanted to go skiing at the Grand Targhee Resort in Alta Wyoming which everybody just calls "Targhee". It is located on the western side of the Grand Teton Mountain and therefore gets a lot of light, fluffy powder snow which is why it is preferred by the locals to the other ski resort in Teton Village on the other side of the Grand Teton Mountain despite having more challenging ski slopes. The only way to get to Targhee, which is about 50 miles from Idaho Falls is through Swan Valley, over the Pine Creek Pass (elevation 6764 feet), Victor, and then Driggs, Idaho. As you leave Idaho Falls to Targhee, there was a sign that says "Don't laugh at the natives." I never understood why it was posted and what the significance was. Proceeding from Driggs, you take a treacherous road to Alta, Wyoming where Targhee is located. Charlie would drive his wife Carol, Dimitri, and myself on Saturdays. Charlie had this mania for wanting to be the first on the ski slopes so we left Idaho Falls at an ungodly early hour. He was on the ski patrol and was supposed to be there in time to ski the hill and knock down cornices before the ski hill opened. To see Dimitri ski was a sight to behold. Charlie and Carol would make it down the mountain in about five minutes. After getting my legs, I could make it in maybe ten minutes. Then when we got down, we would ask "Where is Dimitri?". Then we would look up the hill and there he was. I swear at times it looked like he was skiing *up* the mountain. It would take him the better part of an hour to get down. He had broken his arm slipping on a patch of ice at his home, and ever since he was leery of falling and breaking his arm again. It made for a long day with recuperation on Sundays for work on Mondays.

Together with Charlie and Carol, we had a great time skiing at Targhee. I bought two cars to add to my Corvette which I kept in my garage in the winter because I was afraid to drive it since it had positraction which caused it to slide all over the road and become unstable when accelerating. One car was a Corvair which I used to get to work, and the other was a monstrously large Cadillac which I bought from the real estate broker who sold me my house. This car I let Dimitri use so he could get around by himself. As an investment I bought a small house in Idaho Falls to rent out, and Dimitri helped me move furniture in. The house had two entrances one for the upstairs, and one for the basement which was equipped with a kitchen. I rented out the two floors separately.

Well Dimitri and I were able to get down to serious work right away. He had not waited for his subcontract to begin and had arrived with his notes documenting progress he had made at IGT. What we found would turn out to be the subject of great controversy which even today has continuing ramifications and is not yet completely resolved—we found that the two-phase basic equations possessed complex, i.e., imaginary characteristics!

What follows now is a revised version of Chaps. 7.4 and 7.5 of our chapter in Advances in Transport Processes [15]. I use the material in this form because it traces the evolution of the complex characteristics issue for the reader in a much more logical fashion possible only with the hindsight gained by the passage of time. Generally speaking progress in science is not logical, and I found that out reviewing our progress for this chapter. We were able to produce the characteristic polynomial for Charlie's equations, Eqs. (5.1), (5.1a), (5.2b), (5.2c), (5.4), and (5.4a), for the general case of both phases compressible. It is given in its definitive form,

$$(\lambda + u_i)^2(\lambda + u_j)^2(\alpha_i\rho_j C_j^{-2} + \alpha_j\rho_i C_i^{-2}) - (\lambda + u_i)^2(\alpha_j\rho_i) - (\lambda + u_j)^2(\alpha_i\rho_j) + P = 0. \tag{6.6}$$

This quartic polynomial cannot be factored to solve for the eigenvalues, λ. The other two eigenvalues are the velocities of phases $\lambda = u_i$ and $\lambda = u_j$. We were able to document in a paper prepared for the November 1973 American Nuclear Society Winter Meeting (but never submitted for publication) that imaginary characteristics can result even for the two cases of equal phase velocities and zero relative velocity. The history of this paper will be discussed in Chap. 8.

If both phases are incompressible, Eq. (6.6) becomes

$$(\lambda + u_i)^2(\alpha_j\rho_i) + (\lambda + u_j)^2(\alpha_i\rho_j) - P = 0. \tag{6.7}$$

Equation (6.7) can be factored to solve for two of the eigenvalues as,

$$\lambda = -\frac{(u_i\rho_i\alpha_j + u_j\rho_j\alpha_i)}{\rho_i\alpha_j + \rho_j\alpha_i} \pm \left(\frac{-\rho_i\alpha_j\alpha_i\rho_j(u_i - u_j)^2 + P(\rho_i\alpha_j + \rho_j\alpha_i)}{(\rho_i\alpha_j + \rho_j\alpha_i)^2}\right)^{1/2}. \tag{6.8}$$

which are complex unless

$$P > \frac{\rho_i \alpha_j \rho_j \alpha_i (u_i - u_j)^2}{\rho_i \alpha_j + \rho_j \alpha_i}. \tag{6.9}$$

Thus, at low pressures, there is a possibility that the characteristics are imaginary. This was as far as we could go at this point. Lyczkowski et al. [15] discuss another problem that exists for this set of equations. It has to do with the diffusive force which is associated with the term $P(\partial\alpha_i/\partial x)$. Thus, there already appear to be two problems with Charlie's set of equations.

Charlie became aware of Mecredy and Hamilton's paper [18] which had been published in 1972 and passed the paper on to Dimitri and me. Their momentum equations had the void fraction *outside* of the derivative of the pressure in the momentum equations as in Eqs. (5.2) and (5.2a). This put Charlie, Dimitri, and me into a tail spin since we were under the assumption that his momentum equations were the correct ones. Mecredy and Hamilton performed an analysis involving the Laplace transform of the time variables and a Fourier transform of the spatial variables to obtain the speed of sound as a function of frequency. They had to evaluate a determinant of a matrix which yielded a quadratic for the complex wave number. We proceeded to derive the characteristic polynomial for the Mecredy and Hamilton equations without the added mass term and to investigate limiting cases since they did not perform a characteristics analysis for their equations. However, they were tantalizingly close to the issue of the nature of their equations.

We now turned our attention to analyzing the characteristics for the case of the volume fraction outside of the gradient of pressure. Unfortunately, this changed the rules of the momentum equation ball game. Just what ARE the correct governing theoretical momentum equations? We were stuck at Task 2 in the LOOP Code Development Sheet (Fig. 5.1). We went through the entire characteristic analysis from scratch and found that the characteristics polynomial is given by,

$$(\lambda + u_i)^2(\lambda + u_j)^2(\alpha_i\rho_j C_j^{-2} + \alpha_j\rho_i C_i^{-2}) - (\lambda + u_i)^2(\alpha_j\rho_i) - (\lambda + u_j)^2(\alpha_i\rho_j) = 0. \tag{6.10}$$

which is just Eq. (6.6) with the pressure $P = 0$. Once again, the polynomial does not factor.

For the limiting case of equal phase velocities, the characteristic polynomial Eq. (6.10) factors and the eigenvalues are given by,

$$\lambda = -u \pm C_s \quad \text{and} \quad \lambda = u_i = u_j = u. \tag{6.11}$$

C_s is the stratified speed of sound given by,

$$C_s^2 = \rho_p \rho_m C_m^2 / (\rho_i \rho_j), \tag{6.12}$$

and C_m is the homogeneous equilibrium speed of sound given by

$$C_m^{-2} = \rho_m (\alpha_i C_i^{-2} / \rho_i + \alpha_j C_j^{-2} / \rho_j) \tag{6.13}$$

$$\text{where } \rho_p = \rho_i \alpha_j + \rho_j \alpha_i, \tag{6.14}$$

$$\text{and } \rho_m = \alpha_i \rho_i + \alpha_j \rho_j \tag{6.15}$$

For both phases incompressible, the characteristics are given by Eq. (6.8) with $P = 0$ as,

$$\lambda = -\frac{(u_i \rho_i \alpha_j + u_j \rho_j \alpha_i)}{\rho_i \alpha_j + \rho_j \alpha_i} \pm i \left(\frac{\rho_i \alpha_j \alpha_i \rho_j (u_i - u_j)^2}{(\rho_i \alpha_j + \rho_j \alpha_i)^2} \right)^{1/2} \tag{6.16}$$

where $i = \sqrt{-1}$.

Equation (6.16) shows that the characteristics are imaginary for all nonzero relative velocities, i.e., the characteristics polynomial has complex-valued roots. For single-phase liquid or vapor, the characteristics are real and given by $\lambda_i = -u_i \pm C_i$ and $\lambda_j = -u_j \pm C_j$.

6.2 Characteristics Analyses Using FORMAC

We next turned to Glen Mortensen to help evaluate the characteristic polynomials using a program he wrote using the IBM FORMAC program [17]. This is the same program he used earlier to analyze the stability of difference and iterations equations which were being programmed for the EVET code. This was the only way we could determine the roots of the quartic characteristics polynomials which would not factor. The polynomials were cast into dimensionless form. Figure 6.2 shows the actual plots that the FORMAC program produced. The "R's" represent points in the volume fraction of steam-dimensionless relative velocity plane where the four eigenvalues are real. Where there are no "R's" these are regions where two real and two complex eigenvalues exist. The next step was to trace the boundaries between the real and complex characteristics by hand, annotate them, and then have them drawn as shown in Fig. 6.3a, b.

Dimitri prepared a report documenting our preliminary findings and submitted it to Charlie with a cover letter dated March 26, 1973. This report he says had to be marked CONFIDENTIAL. I looked at the contract and could not find any such demand. There are the usual requests that documents prepared for publication be cleared with the AEC and that they undergo patent clearance. At any rate he did not keep a copy of the results reported except in his head and in his notes. A brief

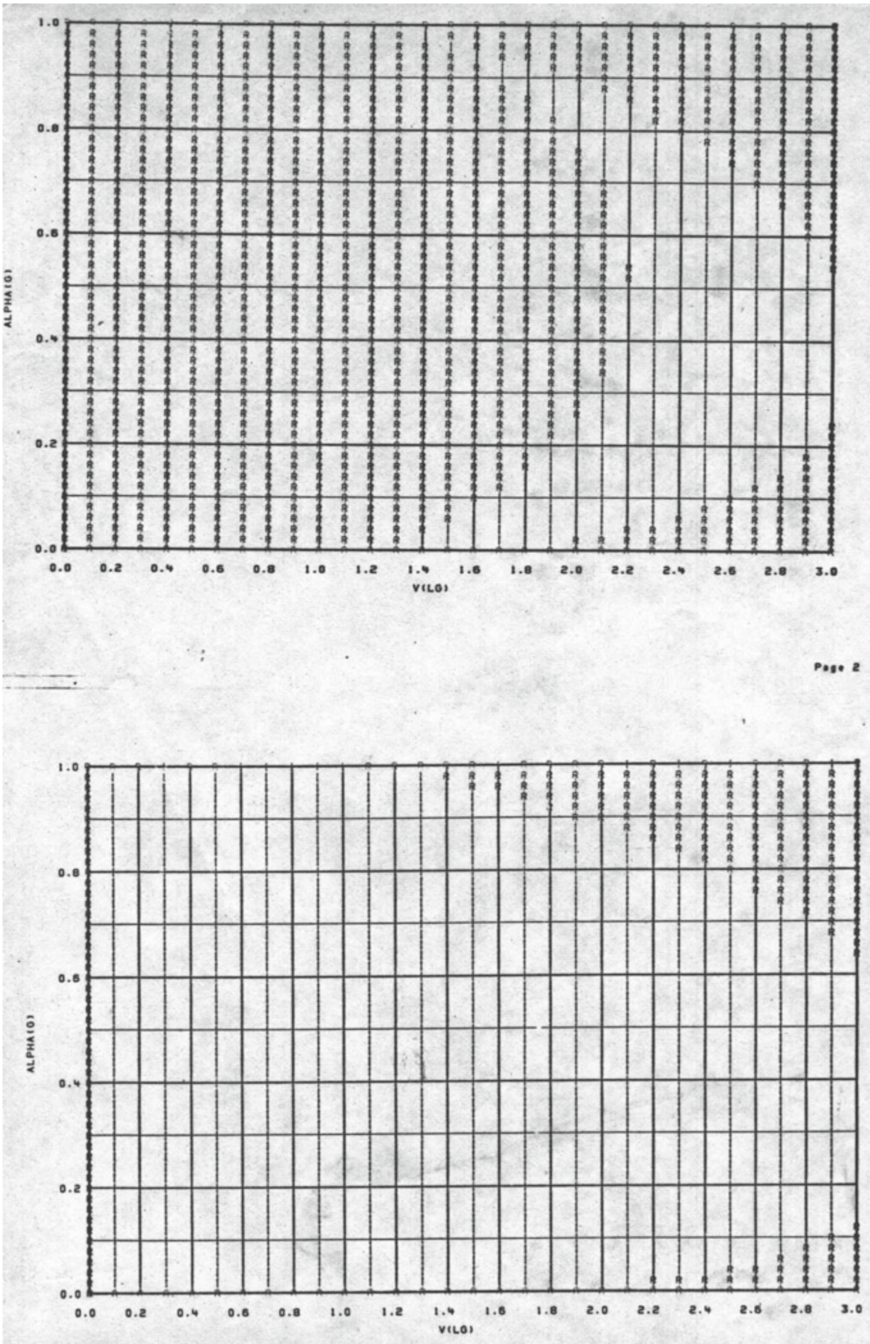

Fig. 6.2 Plots of real characteristics regions (R's) produced directly from the FORMAC computer program [17]. *Top* volume fraction inside the pressure gradient. *Bottom* volume fraction outside the pressure gradient. ALFA(G) is the gas volume fraction and V(LG) is the dimensionless relative velocity [20]

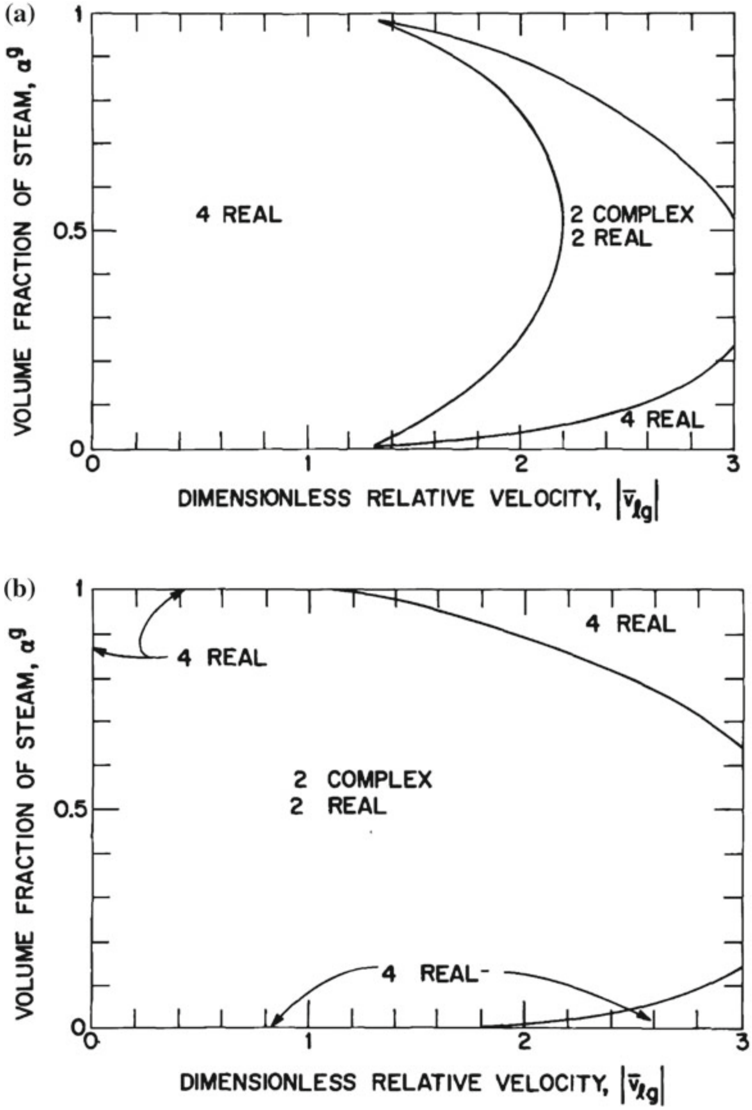

Fig. 6.3 Characteristics maps for volume fraction inside the pressure gradient, Fig. 6.3a, and volume fraction outside the pressure gradient, Fig. 6.3b [20, 23]

summary was reported in Charlie's March 1973 Monthly Management Report of the Analytical Model Development Branch. Apparently by this time only results for the case of the volume fraction inside the pressure gradient were produced shown in the top plot in Fig. 6.2 and in Fig. 6.3a.

Dimitri and I continued to work on the characteristics analysis for the two-phase equations until he left to return to IGT in Chicago as his contract was terminating on August 31, 1973. I was designated by Charlie to approve Dimitri's invoices during the course of his contract. So I was Dimitri's "boss". We made quite a lot of progress from March onward which was reported in Charlie's monthly management reports to Pete Lang.

As the months went by many more cases including two forms of the transient flow forces were analyzed for the two-phase equations using Glen Mortensen's FORMAC computer program. It was possible to evaluate these cases using realistic steam tables, such as those developed by the ASME. They are slow running but very accurate. In June 1973, we wrote a five page report summarizing the progress that had been made up to that point on the characteristics analysis of the basic equations described in this chapter. This report was incorporated into Charlie's June 1973 monthly management report [19] and served as a draft for an abstract prepared for the November 1973 American Nuclear Society (ANS) Winter Meeting to be held in San Francisco.

In July, we submitted the abstract to the technical program chair, Dr. S. A. Bernsen from Bechtel Power Corporation. The only review that it received came back stating that the abstract was too long. It had to be within the 600-word maximum length, including figures, tables, and graphs. It also raised the questions "Is it certain that Wallis' leaving α_i outside the gradient was not typographical? Is there any physical basis for the existence of an imaginary region?" We revised the abstract and resubmitted it on August 21. It was accepted shortly thereafter on August 30 and appeared in the Transactions in November [20]. The figure in the abstract is for the case of phase volume fractions inside the gradient of pressure. It is only near the end of the abstract that we stated that for the case of the phase volume fractions outside the gradient, "… for nonzero velocities, the characteristics are all imaginary…except for equal velocities and single-phase flow." This is to my knowledge, the first published account reporting the existence of imaginary characteristics for *both* of these two sets of two-phase equations. Unfortunately, the abstract gives the impression that we are recommending the case of the volume fraction inside the gradient of pressure. As mentioned in Chap. 5, I was able to show in an unpublished memo that with the volume fraction inside the derivative with the pressure, unrealistic results would result [21]. This and an order of magnitude analysis were the reasons that the momentum equations being programmed for the SLOOP code development for the UVUT code were in the form of Eqs. (5.2) and (5.2a), rather than Eqs. (5.2b) and (5.2c) even though they had imaginary characteristics in regions of interest for simulations.

The manuscript that Dimitri and I prepared during the summer months of July and August and into early September with the title "One-Dimensional Two-Phase Flow Equations and Their Characteristics" was intended for our presentation at the November 1973 ANS Winter Meeting was quite comprehensive and documented everything we had learned and analyzed up to that point including some of the analysis included in Sect. 6.1, however in dimensionless form. The authors of this paper were in order: Dimitri, myself, Charlie, and Dan Hughes. It contained a cleaned up map for the case of the momentum with the phase volume fractions outside the pressure gradient (Fig. 6.3b) shown in its raw form in the bottom of

Fig. 6.2 and a revised version of the map for the case of the phase volume fractions inside the pressure gradient (Fig. 6.3a) which appeared in our abstract [20]. The first map was not included in our abstract; there was only the terse statement quoted in the previous paragraph. In addition, it also contained additional characteristic maps for two forms of the added mass from the literature for both form of the momentum equations. All of these characteristic maps as well as for many more cases were generated using Glen Mortensen's FORMAC computer program and were first documented in an interoffice correspondence report to Charlie in October 1973 [22]. Most of the results in this report have never been published. For some reason unknown to me, we never submitted our paper for publication to the ANS journal Nuclear Science and Engineering. By this time, we had found additional literature dealing with the two-phase equations for fluidization as well as obscure two-phase flow papers from the Soviet Union. I should point out that two of these references were included in our abstract [20]. I traveled to San Francisco in November to present the paper. I should mention that the references to the fluidization and obscure Russian literature must have appeared in my presentation slides. By the way, they also appeared in Harlow and Amsden's first 1975 paper [23] submitted for publication in early 1974.

A pivotal event occurred during Dimitri's sabbatical. Victor Ransom had a friend that joined ANC as things were beginning to turn sour at Aerojet General Corporation in Sacramento California with layoffs beginning to occur. He encouraged Vic to apply to ANC in Idaho Falls which he did. He was interviewed by Larry Ybarrondo in early 1973 and was subsequently hired. He joined me in the System Model Development Section. Being an Idaho native, it would be a return to his roots. Vic, born in Idaho in 1932, graduated from the University of Idaho in 1955 with a B. S. degree in Chemical Engineering. He then joined North American Aviation in Canoga Park, California where from 1955 to 1959 he developed transient simulation methods for liquid rocket engines and computer programs for the analysis of supersonic rocket engines using the method of characteristics. In 1959, he joined Aerojet General Corporation in Sacramento, California where he was appointed supervisor of Aerojet's fluid mechanics and heat transfer groups. He continued to apply his expertise to supersonic nozzle design and simulation of liquid rocket systems. In the evenings during his employment at Aerojet, Vic would take graduate courses at Sacramento State University. In 1965, he decided to continue his education formally and enrolled at Purdue University in West Lafayette, Indiana. Under his doctoral thesis advisor, Professor Joel D. Hoffman, he developed one of the first computer programs using the method of characteristics to analyze three-dimensional supersonic nozzle flow problems. After he graduated in 1970 with a Ph.D. in Mechanical Engineering, he returned to Aerojet General in Sacramento to work on supersonic flow problems for NASA's space program. His experience in numerical methods, computer program development, and the method of characteristics and made him a valuable addition to the section.

After my ad hoc stint as Section leader, Glen Mortensen stepped in for me since I was working intensely with Dimitri. He took over writing up the portion of progress for the System Model Development Section and Bill Yuill, Leader of the Correlation Development and Material Modeling Section, would write up progress for the SLOOP code correlation development. Then in July, 1973 Vic was appointed to fill the vacancy that Charlie had created when he left as leader of the System Model Development Section to become Manager of the Analytical Model Development Branch.

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Chapter 7
The SLOOP Code Development

Nomenclature

Roman Letters

C Speed of sound
g Gravitational acceleration
K Drag function
P Pressure
u Velocity in x direction
t Time
x Coordinate direction

Greek Letters

α Volume fraction
λ Eigenvalue of the characteristic polynomial = dx/dt
ρ Microscopic material density

Subscripts

i Phase i = solid or liquid
j Phase j = gas or vapor

This chapter is sandwiched between Chaps. 6 and 8 which deal with the issues of the discovery of complex characteristics and their analysis and about the publication history of the characteristics paper [1]. Those chapters describe a major event in the SLOOP code project that spanned the roughly three and one-half years of the project's existence from its initiation in 1972 to its explosive conclusion in 1975 and in the years beyond its demise. Unfortunately, theoretical equation development was supposed to be just a very minor aspect of the project as the first page of the LOOP code development sheet shows in Fig. 5.1. In fact, the characteristics analysis wasn't even listed as a task and certainly wasn't anticipated or planned.

R.W. Lyczkowski, *The History of Multiphase Science and Computational Fluid Dynamics*, Mechanical Engineering Series,
https://doi.org/10.1007/978-3-319-66502-3_7

There were no fall-backs or safety nets (commonly called Go-No Go's) built into ANC's program (or project) evaluation review technique, commonly abbreviated as PERT, network chart. I don't recall and certainly don't have a copy of any modifications beyond the first one approved in March 1973 created for the LOOP code. The descriptors LOOP code, SLOOP code, and advanced LOOP code were all used interchangeably to describe the project designed to replace RELAP4. Optimism and grand promises may have sold the project to the AEC, but lack of foresight flawed its completion. Nonetheless, there were a lot of significant activities going on in which I was not personally involved. Because of my preoccupation with the characteristics problem, I was not very familiar with them at the time. Most of these activities were directed at getting the many pieces together in order to develop an increasingly complete, realistic, and reliable advanced LOOP code. I will also explain the reasons why the project failed including, as delicately as possible, the role that the politics of science played as perpetrated by the NRC. Even though the SLOOP code project did fail, the groundwork and experience were invaluable to future code developers either directly or indirectly. The most obvious direct beneficiary was the legacy passed on to Vic Ransom, John Trapp, and Dick Wagner who would go on to develop the RELAP5 computer program which turned out to be a smashing success. The origin and summary of RELAP5 will be discussed in Chap. 10. Little of the achievements of the SLOOP code were documented in peer-reviewed open-literature publications, and up to now, as mentioned in the Preface, no history of this project has ever appeared. Fortunately, the Electric Power Research Institute (EPRI) funded a project at Energy, Inc., in 1976 to document a significant portion of the SLOOP code effort and achievements in a three-volume publication authored by a portion of the SLOOP code investigators, including myself [2–4]. Unfortunately, I can only include in this chapter highlights of some of the others, concentrating on the ones to which I contributed directly on the tasks assigned to me.

Computer programming continued for the UVET and UVUT equations in 1973 and into 1974. The instabilities first experienced with the EVET equations programmed into the EVET code mentioned in Chap. 6 reared their ugly head in new guises. This slowed down the project's progress significantly to achieve the SLOOP code's lofty goals and many tasks some of which are shown back in Chap. 5 in Figs. 5.1 and 5.2. Each member of the project had their own opinion as to what was causing these instabilities, and hit and miss fixes were employed. However, instabilities persisted. I postulate that the sources for the instabilities can be categorized into two types: (1) modeling of the two-phase equations and (2) numerical problems with the finite-difference equations. Of course, there was always the possibility of "bugs," i.e., coding errors.

Let's look first at category (1) for potential sources of instability. I cannot be absolutely certain, but I think that the first set of two-phase equations programmed into what was internally called the STUBE (Seriated Tube) code were Eqs. (5.2b) and (5.2c).These equations were found in Chap. 6 to be hyperbolic, at least in regions of application for nuclear reactor safety analysis. This "test-bed" code was "barebones" since not all of the correlations for friction, heat transfer, and flow regimes were yet programmed and checked out in auxiliary codes such as EVET, UVET, and ZVUT to be discussed shortly. Since no one in the group doing computations (including myself) had any previous experience with the physical behavior of these particular two-phase equations, “baby steps” were taken using very small pressure drops to accelerate the phases using gentle transients. An order of magnitude analysis showed that even though these equations were hyperbolic over a considerably large range, their computational behavior for realistic safety blowdown analysis simulations would have been catastrophic where pressure drops cover the range from approximately 7 to 0.1 MPa, atmospheric pressure. This would result from the overpowering effect of the terms $P\partial\alpha_i/\partial x$ and $P\partial\alpha_j/\partial x$. When we found other investigators, for example Mecredy and Hamilton [5], using the equation set, Eqs. (5.2) and (5.2a), which were found in Chap. 6 to have complex characteristics and hence ill-posed, the switch was made to have the computer program to have both sets of these equations as options. It also instigated us to add transient flow forces [1, 5]. Since we were deep into the characteristics investigation to find a set of UVET and UVUT equation sets that were hyperbolic, this type of instability was ascribed to the complex characteristics and spurred us to find alternative equations which had real characteristics. Some of this effort will be reported in this chapter. Another potential source for instability problems might have originated from the energy equations discussed in Chap. 5. Early on, they were missing the terms $P\partial\alpha_i/\partial t$ and $P\partial\alpha_j/\partial t$ in the energy equations in internal energy form. Dimitri first showed for the case of the volume fraction outside the pressure gradient that these terms must be present [6]. He later derived the energy equations from first principles [7, 8] to show that such terms must be present in the energy equations. He showed in reference [7], pages 278–280, that without these terms the energy equations could result in a violation of the entropy inequality.

Now let’s look at category (2) for potential sources of instability. As mentioned early in Chap. 6, the overarching ground rule was to use fully implicit central differences for spatial derivatives because this numerical method is unconditionally stable, at least for the diffusion equation [9]. However, it turns out that LASL Group T-3 routinely used upwind differencing which introduces a great deal of numerical diffusion to help damping of potential instabilities. LASL wasn’t particularly interested in accuracy of their computation since they weren’t yet into quantitatively analyzing experiments. Either we were unaware of this or were locked into central differencing and no artificial viscosity on a philosophical level imposed by Charlie, who was an idealist at heart. The same argument can be made for the use of artificial viscosity that LASL uses routinely to stabilize their numerics. Charlie wanted as high fidelity as possible for the physics without introducing inaccuracies resulting from non-physical damping terms. The very ordering and treatment of which terms to update in the iteration scheme will effect convergence. This was analyzed exhaustively by Glen Mortensen using the FORMAC software [10] using what he called the STAB code. Then there is the question of properly posed boundary conditions. This is an area where the “art” of numerical modeling is involved. As one of our teachers at IGT admonished us, boundary conditions must be real/physical and not contrived. A great deal of effort was poured into the treatment of boundary conditions, not only for two-phase simulations using the STUBE code but also in the single-phase EVET code. If something didn't work for single phase, it surely wouldn't work for two-phase.

In the middle 1960s, Herbert Kouts was Chairman of the Advisory Committee on Reactor Safeguards (ACRS) for the AEC. Then, in the early 1970s he became Director of the AEC's Division of Reactor Safety Research (RSR) and held this post until its successor was appointed, even after the NRC was formally initiated in 1975. In this position, he visited the SLOOP code group at least once around April 1974 to review progress. I am quite sure the discussion of the continuing issue of the complex characteristics was on the agenda. The meeting was considered a success by upper management. ANC's President, Charles Leeper, also had at least one meeting with the section. I remember very clearly that as he sat listening to the presenters, he would dangle his tea bag as he looked on at us with glassy eyes. Kouts hired L.S. Tong directly from Westinghouse in 1974, putting him in direct control of the LOOP code work. For reasons to be discussed later in this chapter, it soon became clear to Charlie that Tong's every intention was to dismantle the SLOOP code work. In 1977, Tong and G.L. Bennett reviewed the NRC water reactor safety program without even an indirect reference to the SLOOP code effort [11]. They do mention results obtained by LASL using the fledgling SOLA-DF code. Internally, we were concerned because the UVUT code kept blowing up unexpectedly and repeatability in the transition from single-phase to two-phase flow trying to simulate Standard Problem 1 based on the Edwards and O'Brien experiment [12]. The resolution of this problem will also be discussed later in this chapter. Such Standard Problems were part of the Cooperative Analyses of Standard Problems (CASP) program sponsored by the AEC with the cooperation of the major US nuclear reactor and fuel manufacturers. The SLOOP code schedule was slipping, and we were under pressure to meet the schedule and deadlines imposed by the NRC. This problem would soon become evident to the sponsor.

In July, 1973 Vic Ransom was appointed to fill the vacancy that Charlie had created when he left as leader of the System Model Development Section to become Manager of the Analytical Model Development Branch. Vic allowed me to copy two of his Record notebooks which he kept while at ANC. Although he started employment early in 1973, the entries don't start until the middle of November 1973, fully four months after his appointment as Section leader. They continue until nearly the middle of 1980. These notebooks helped me somewhat to explain what was really happening (or NOT happening) during the SLOOP code development. Vic and I became close friends as soon as he joined me in the System Model Development Section. We remained friends even after I left ANC to join Energy, Inc., in 1975. We would go skiing together with his wife Delrie at Targhee. He was and still is an excellent skier, much better than I. We have remained friends all these decades.

7.1 Dimitri's Contract Is Extended

On October 1, 1973, Charlie, now Manager of the Analytical Model Development Branch, wrote an interoffice correspondence to Pete Lang, now Manager of the TRSP, proposing to extend Dimitri's contract from January 1, 1974 to June 30, 1974. The initial contact which was drawn up for Dimitri's sabbatical described in Sect. 6.1 was from February 15 to August 31, 1973. The SLOOP code was in trouble (although the sponsor was kept in the dark), and we needed Dimitri's continued assistance. In this letter, Charlie's justifications were numerous. He stated that the "Basic equations had been determined [!]…" and "We desire…to determine why the one-dimensional equations are not hyperbolic in all regions." He then summarized some of Dimitri's accomplishments including his "…completely novel method for rationally deriving the basic…UVUT two-phase flow equations…to see if the Second Law of Thermodynamics is satisfied for the mixture." "Based on his studies, he suggested the addition of terms to the UVUT energy equations which will now enable us to solve problems in all regions of practical interest.[!]" Charlie also cited Dimitri's familiarity with the Russian literature to supply information to the LOOP code developers. Dimitri's "…work would fall mainly under Task 10 on the LOOP Code Development MBO [see Fig. 5.1] 'Review of code against standard test problems and modification if necessary'." The amount of effort would amount to a six month maximum of full-time effort and three round trips from Chicago to Idaho Falls. The modification to the original Agreement was sent to Dimitri January 11, 1974, for approval which he signed, witnessed again by Darsh Wasan, and it was returned by January 31, 1974. Considering the slippage in timing, the expiration of the modified Agreement might have extended past June 30, 1974.

7.2 Comparison of Prototype Two-Phase SLOOP Code with Analytical Solutions

Both during and between Dimitri's visits to ANC during his sabbatical in 1973 and subsequent contract extension in 1974, we would formulate and work on analytical solutions. With his guidance, I would devise "proof of principle" simulations for the two-phase equations in the EVET, UVET, and UVUT codes for problems that could run, especially those that could be compared with literature results. The two-phase equations truly fascinated me and I wanted to find out how they performed and what they could predict.

I will now give just a few examples of the kind of solutions and applications I devised to validate the EVET and UVET computer programs. These were two of the auxiliary programs which were developed, but not meant as a final product to shake down solution (iteration) schemes, boundary condition treatments, and prototype correlations. The first set of three analyses involved comparison with analytical solutions and independent calculations for horizontal pipes [13, 14] and vertical pipes [15] and were performed early on in 1972 and 1973. The horizontal pipe analysis was performed using the EVET and UVET codes using constant and variable wall friction factor given by the Blasius equation [13, 14]. The vertical pipe analyses were performed with both the EVET and UVET codes with a constant interphase drag function, without and with wall heat transfer [15]. Some of these results were collected together and published years later in the AIChE journal while I was at Lawrence Livermore Laboratory (LLL) [16]. While I was there, I was given wide latitude concerning what I could do. In fact, anything involving multiphase flow was considered part of my job. This paper showed conclusively that phase separations and flow reversals were possible in vertical pipes and could therefore be possible to compute in pressurized water-cooled nuclear reactor downcomers and cores during a LOCA transient undergoing emergency core cooling (ECC) [16]. The reason I spent a lot of time on this particular problem and decided to publish the results later was because it vindicated Charlie's argument to the AEC in 1970 as discussed at the end of Chap. 4 that with the two-phase equations he proposed, such phenomena would be possible to describe and would be impossible to describe using existing safety codes such as RELAP3 which used single-phase equations. For this reason, I included Charlie as coauthor. In the report first documenting the vertical pipe simulations [15], I used a technique to convert two coupled first-order differential equations for the two phases into two decoupled second-order differential equations and obtained analytical solutions. I must have learned this technique at IGT either when I took Dimitri's courses IGT 510 Engineering Calculations and IGT 516 Numerical Methods In Transport Phenomena (in which Charlie assisted Dimitri) or gotten it from Dimitri when he was consulting for ANC. In any case, I did not include the results in the AIChE paper even though the results agreed qualitatively with the simulations.

The next two analyses [17, 18], which remain unpublished, concerned the depressurization of an ideal gas to compare the EVET code results with the theoretical MOC calculations I performed [17] and with the result published in Rudinger's book [19] first presented in reference [18] and then in more detail in Appendix III-A in Volume II of the EPRI report [2]. The study contained in the first report [17] which gives details of the simulation was used to show that full compressibility could be accounted for, that numerical dispersion could be assessed, and that self choking at sonic velocity at the pipe exit could be predicted for the EVET code. Figure 7.1 shows he results of this study which was prepared for one of the presentations to the NRC. The code results (wavy curve) for the velocity at the pipe exit are compared with the first two plateaus independently computed using the MOC. Without any friction, many oscillations were computed at these plateaus due to the Gibbs phenomenon inherent in the low-damping central differences used in the EVET code. With friction, these oscillations were almost entirely eliminated as shown in Fig. 7.1. This figure also shows the approach to steady state with a small overshoot at around 0.1 s. The second study was used to compare with the calculation shown in Rudinger's book which the reader is encouraged to consult [19]. This required the development of computational boundary condition treatment at the exit of the pipe during outflow from the pipe and during flow reversal. Details of the simulation are given Appendix III-A in Volume II of the EPRI report [2], pages A-19 to A-27. Figure III-A-7 on page A-25 [2] shows the comparison for the pressure response at the closed end of the pipe for the first roughly 30 ms. After the initial rarefaction wave travels to the closed end and is reflected to the outlet, the flow reverses at about 1.5 ms. It then continues a damped oscillation until the pressure in the pipe subsides to the outlet pressure. As can be seen, the agreement is excellent except for some numerical damping at about 0.5 and 2.0 ms. I have to apologize for the quality of Fig. 7.1 which is a scanned copy of the original [17] and for the use of English units which were the only ones used in the early 1970s in the nuclear industry.

Now, we arrive at the so-called water faucet problem. There is a misconception in the open literature [20, 21] that the water faucet test problem originated with Ransom [22]. I want to set the record straight. The fact of the matter is that I devised this problem in 1973! [23]. The idea behind this thought problem was similar to that for the gravity dominated flow problem described above which predicted countercurrent flow and flow reversal in the downcomer or core of a pressurized water nuclear reactor and was published in the AIChE Journal [16].

The water faucet problem is an idealization of the flow of a column of water falling freely under the effect of gravity. The steady-state solutions are extremely simple and are given by,

$$\mathrm{v}_l\,(x) = \sqrt{\mathrm{v}_{lo}^2 + 2gx} \tag{7.1}$$

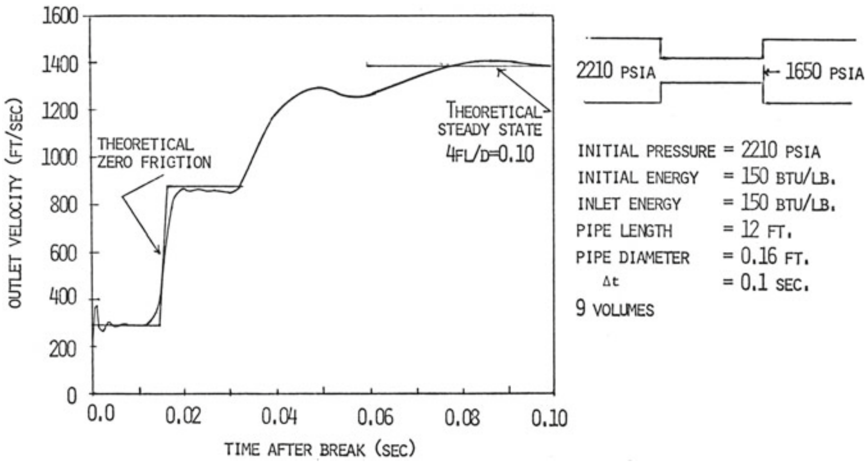

Fig. 7.1 Outlet velocity plot for decompression of an ideal compressible gas [17]

and

$$\alpha_l(\mathrm{x}) = \alpha_{lo}\mathrm{v}_{lo}/\mathrm{v}_l(\mathrm{x}) \tag{7.2}$$

where v_{lo} is the inlet water velocity, v, α_{lo} is the inlet water volume fraction, α_l, g is the acceleration due to gravity, 9.8 m/s^2, and x is the distance along the pipe. The effect of interfacial friction and pressure changes is assumed to be negligible. Figure 7.2 is a scan of the transient solution performed by the UVET code as shown for the first time at one of the AEC review meetings in ANC fiscal year 1974 which extended from July 1, 1973 to June 30, 1974. The inlet and initial velocities of the water are 10 ft/s, and the length of the pipe is 6 ft. The inlet and initial volume fraction of water is 0.5. At time t = 0^+, gravity is turned on and the water column begins to neck down and eventually reaches the exit at the bottom and a steady state is reached. The necked down region travels at the velocity of the water column, 10 ft/s. Comparison of the analytical solution given by Eq. (7.1) with the UVET code results was actually included in the ASME preprint for the 1975 ASME Winter Annual Meeting held November 30–December 4, in Houston, Texas [24] and in the characteristic publication in 1978 [1]; however, the details of the simulation were not given. The history of these two publications will be discussed in Chap. 8. The simulation details were presented in Volume III of the ERPI report [3], pages 8 through 18, with a cleaned-up version of Fig. 7.2 in Fig. 2.3. In 1974, I analyzed the effect of interfacial drag on the steady-state by numerically solving the coupled ordinary differential equations, but was never published [25]. A cleaned-up version of Fig. 7.2 together with more details of the analysis appeared in Volume III of EPRI-NP-143 [4]. It was never published in a peer-reviewed journal. I extended the water faucet problem to assess the effect of adding the terms $P\partial\alpha_i/\partial x$ [23]. The effect proved catastrophic and should have definitely eliminated this equation set from further consideration with these terms in the momentum equation given by Eqs. (5.2b) and (5.2c). Unfortunately, this analysis was never published. Thus, the water faucet problem is an extremely simple yet sensitive model to assess two-phase model momentum equations modeling just as Ransom and Hicks [26] observed with their transverse momentum formulation.

Ransom formulated his water faucet test problem as a contribution to a number of numerical benchmark tests presented at a workshop on two-phase flow fundamentals sponsored by the Council on Energy Engineering Research in 1984 and published in 1987 [22]. The results of this workshop were envisioned to eventually be used by the Office of Basic Energy Sciences of the DOE. The avowed purpose of such tests was to compare and assess the various solutions to two-phase equations solved by numerical methods, to establish which are most reliable, and to give guidance to users of two-phase computer models. In that sense, they are similar to the standard problem series sponsored by the AEC mentioned earlier. Earlier in 1984, Ransom and Hicks [27] either consciously or unconsciously used the very same water faucet problem reported in the EPRI report [4] without any reference to assess their transverse momentum two-phase two-pressure model [26]. The numerical benchmark version of the water faucet problem definition was different

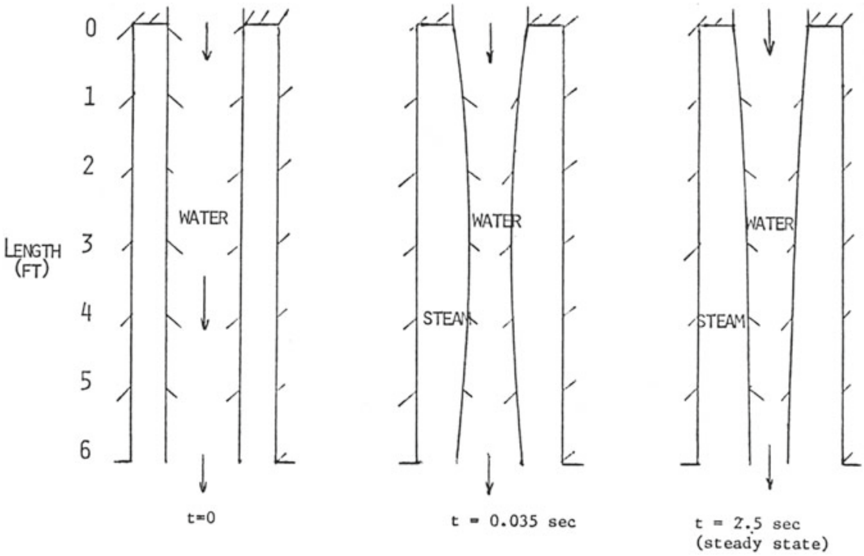

Fig. 7.2 Water faucet simulation showing the necking down of an initially uniform column of water [3, 23]

specifying an inlet and initial water velocity of 10 m/s and an inlet and initial water volume fraction of 0.8. This problem has become a benchmark for two-fluid, i.e., seriated continuum two-phase models [20, 21]. The analytical solution for the transient was given in reference [20] with no derivation. The solution was derived using the method of characteristics in 2017 [27]. The water faucet problem displays a “contact discontinuity” at the point of necking down not observed in Fig. 7.3, nor in Volume III of the EPRI report [4] most likely because of the very course mesh consisting of only nine finite-difference nodes. Even with this course mesh, computational times were long in the early 1970s, and so a mesh refinement study was not practical.

7.3 Attempts to Develop Two-Pressure Models Having Real Characteristics

This section will give the reader a flavor of some of the efforts which have been expended in developing or devising hyperbolic two-phase equations having all real characteristics. Because of the problem with the early proposed two-phase equations not being totally hyperbolic except in limiting cases as discussed in Chap. 6, an effort began very in the SLOOP code project to formulate an alternative equation set or equation sets which would be completely hyperbolic. One of the first such models was devised by Ramshaw and Trapp for Dimitri’s Roundtable Discussion

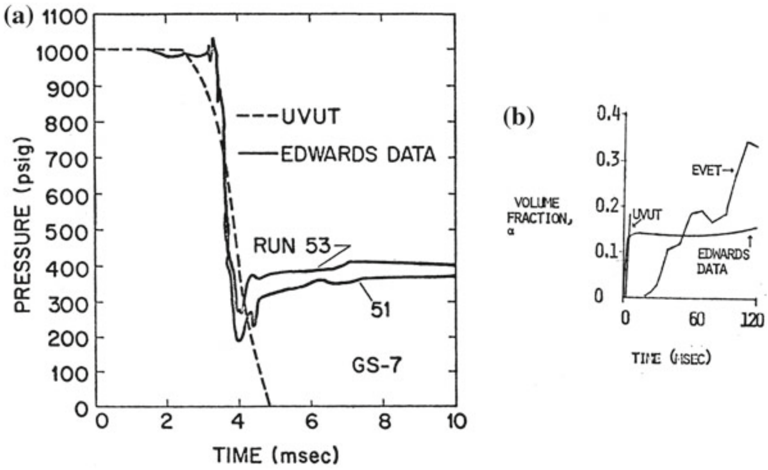

Fig. 7.3 UVUT code simulation of standard problem 1. **a** Pressure at measuring station GS-7 near the closed end of the pipe. **b** Steam volume fraction at measuring station GS-5

[28]. It is a two-pressure model with the inclusion of surface tension relating the two pressures. A report amplifying Ramshaw and Trapp's analysis appeared in 1976 and was eventually published in 1978 [29]. The momentum equations are identical to Eqs. (5.2) and (5.2a) with the addition of subscripts on the phase pressure given by P_i and P_j. The pressures are then related by the expression

$$P_i - P_j = -\sigma H(\partial^2 \alpha_i / \partial^2 x^2) \tag{7.1}$$

where σ is surface tension and H is the spacing between parallel plates. The continuity equations are given by Eqs. (5.1) and (5.1a) and thus remain unchanged.

Ramshaw and Trapp determined the characteristic eigenvalues, μ, given by $\mu = 1/\lambda$ because the **A** matrix is singular, see Eq, (6.3), $\mu = 0$ (counted two times), $\mu = (u_i \pm C_i)^{-1}$, and $\mu = (u_j \pm C_j)^{-1}$. They also performed a linear stability analysis of their equations and developed the relationship between characteristics and linear stability probably for the first time. Unfortunately, they found that the value of the physical value of surface tension is too small to stabilize small amplitude disturbances on the order of the mesh spacing in a finite-difference numerical scheme and so they advocated the use of artificial surface tension.

I formulated another hyperbolic two-phase equation set inspired by the Rudinger and Chang publication [30]. Their equations can be considered to be a "dusty gas" formulation since they do not contain the volume fraction of the dispersed solids phase. The entire pressure gradient is contained in the continuous gas phase. Thus, the model is applicable only for the flow of extremely dilute suspensions of particulate solids. The equations are hyperbolic with the eigenvalues given by u, v (counted 3 times), and u ± a where u is the gas velocity, v is the solids velocity, and a is the speed of sound in the gas phase. They then solved a problem involving a depressurization of a gas-solids mixture using the wave-diagram technique. I extended the Rudinger and Chang model in 1974 [31] and then used it to analyze pressure propagation data in a 1975 conference presentation which was not published until 1978 [32]. The generalized Rudinger–Chang momentum equations are given by,

$$\frac{\partial}{\partial t}(\alpha_i \rho_i u_i) + \frac{\partial}{\partial x}(\alpha_i \rho_i u_i u_i) + \frac{\partial P}{\partial x} - K(u_j - u_i) + \alpha_i \rho_i g = 0 \tag{7.2}$$

$$\frac{\partial}{\partial t}(\alpha_j \rho_j u_j) + \frac{\partial}{\partial x}(\alpha_j \rho_j u_j u_j) - K(u_i - u_j) + \alpha_j \rho_j g = 0 \tag{7.2a}$$

The continuity equations remain unchanged from Eqs. (5.1) and (5.2). Comparing Eqs. (5.2) and (5.2a) with Eqs. (7.2) and (7.2a) reveals what has happened to the pressure gradients for the two phases. As can be clearly seen, the above equations constitute a degenerate two-pressure model with the second-phase pressure equal to zero. With the simple expedient of placing the entire pressure drop in the continuous phase, defined by Eq. (7.1), the equations become hyperbolic with the eigenvalues, λ, given by $\lambda = u_i$, $\lambda = u_j$, $\lambda = u_i + \sqrt{\rho_m C_m^2/\rho_i}$ and $u_j + \sqrt{\rho_m C_m^2/\rho_j}$ where C_m and ρ_m are defined by Eqs. (6.13) and (6.15). However, a logical problem results. What constitutes the continuous phase? One possibility is to switch which phase carries the entire pressure drop at a volume fraction equal to one half.

A very expedient "fix" is to add the one-dimensional viscous terms to the momentum equations given by Eqs. (5.2) and (5.2a). This was suggested as far back as 1973 in Charlie's August monthly management report. This simply entails adding the terms $\mu_i(\partial^2/\partial^2 x^2)$ to each momentum equation. I don't know if this suggestion was actually programmed into the UVET or UVUT codes. In any case, the equations become degenerately hyperbolic. The characteristics were obtained in 1980 by Arai [33]. The eigenvalues, λ, are $\lambda = 0$ (taken four times), $\lambda = u_i$, and $\lambda = u_j$.

Vic Ransom started to develop what he termed the transverse momentum two-phase model as far back as 1973 shortly after he joined ANC and settled into the System Model Development Section [34]. He refined this model over the years and in 1980 published the resulting analysis with Hicks [26]. This equation set is hyperbolic, and the eigenvalues, λ, are given by $\lambda = (u_i \pm C_i)$ $\lambda = (u_j \pm C_j)$, and $\lambda = (u_i + u_j)/2$. They analyzed the effect of the transverse velocity on the steady-sate solution to the water faucet problem discussed in the previous section and found less than satisfactory results.

Lee and Lyczkowski [35] analyzed four two-phase equation sets, including the generalized Rudinger–Chang set discussed above, which are hyperbolic. What we did at my recommendation was to compare the performance of these various equation sets by numerically solving three problems: batch settling, a fluidized-bed experiment, and a jet impingement experiment. All of the five equation sets, including the basic set given by Eqs. (5.2) and (5.2a) which is non-hyperbolic in one dimension, gave the essentially the same results for all three problems except tor the fluidized-bed experiment. In my opinion, this is the most rational way to discriminate between proposed equation sets rather than to idly argue over the merits of each equation set. Even though the study is not entirely definitive, it is a start.

The added mass terms analyzed in the characteristics paper [1] might have made the two-phase equations hyperbolic, but the limited analysis performed did not find that that such terms rendered the eigenvalues totally real. Stadke [36] extended the added mass term to develop his hyperbolic equation set to be discussed in Chap. 8.

A so-called bubble growth term was reported in Charlie's January 1974 monthly Management Report following the work of Boure et al. [37] which was claimed to render the two-phase equations totally hyperbolic, but I don't find any proof of this claim. It was subsequently added to the UVUT and probably the UVET codes. It is given by,

$$C_\alpha \frac{\alpha_g \alpha_l \rho_g \rho_l}{\alpha_g \rho_l + \alpha_l \rho_g} \left(u^g - u^l\right)^2 \tag{7.3}$$

where C_α was probably taken to be 0.5. Equation (7.3) is then added and subtracted from each of the two momentum equation, one for the vapor and one for the liquid so that their sum adds to zero.

7.4 Summary of SCORE, SPLEN, Executive, ZVUT, EVET, UVET, ADF, SSUVET, and UVUT Codes

As the reader can surmise from all of the above, 1973 going into 1974 was an extremely busy and hectic period. Throughout 1972 and into 1974, there was little if any intervention from the AEC sponsor. The SLOOP code project was trying to do the best it could to keep a modicum of progress going in spite of horrendous problems with the characteristics issue and numerical stability problems. Development of the SCORE (Seriated Core), SPLEN (Seriated Plenum), and executive codes lurched forward as well, and the auxiliary computer programs EVET, UVET, UVUT, and ZVUT designed for development of the SLOOP code were continuing to come together. Reporting started to bulk up a little after Vic became leader of the System Model Development Section in July 1973 and more so when he became Manager of the Analytical Model Development Branch in February 1974 replacing Charlie, who then exchanged places with Vic and returned as Section Leader. I took over the reporting for the LOOP code activities. Dan Hughes basically took over reporting for the core and plenum codes, Bill Yuill continued to be in charge of correlation development, Glen Mortensen continued to develop the executive code, and Dick Farman was in charge of the model development experiments. These were the pieces which were supposed to be integrated together to produce the advanced LOOP code. Too many pieces too little time considering the basic problems with the characteristics and numerics.

As already mentioned throughout this chapter, the EVET, UVET, and UVUT codes were written as auxiliary test beds for developing finite-difference and iteration schemes including boundary conditions and for evaluating various terms added to be basic two-phase momentum having complex characteristics as well as the energy equations. The LOOP (SLOOP), core (SCORE), and plenum (SPLEN) codes were to be unequal phase velocity and unequal temperature codes to describe the behavior of all components of a nuclear reactor system during a LOCA. The purpose of two others the ZVUT and ADF codes has not been described. The executive code was supposed to control the integration of all these codes and to interface them with the user. These codes are all a part of the SLOOP code development effort and each had a definite purpose and objective. Brief descriptions of these components will now be given.

Core Code (SCORE)

The objective of the core code (SCORE) is to develop the three-dimensional distribution and state of the coolant within the core of nuclear reactors during transient incidents, including a LOCA. The effects of subchannel cross flow, mixing caused by partial channel blockage and free convection flow and heat transfer will be calculated. It was intended that unequal velocity and temperature equations would be employed, but it never got beyond a compressible equal velocity and equal temperature with two-phase flow friction multipliers and void fraction correlations. I should mention that Walter Wnek, a graduate of IIT from the Department of Gas Technology in 1973, was hired to work on this code with John Ramshaw, John Trapp, and Dan Hughes. Therefore, there were a total of four Gas Technology graduates working on the SLOOP code project!

Plenum Code (SPLEN)

The objective of the plenum code (SPLEN) is to develop turbulent two-phase flow in regions of the nuclear reactor system where multi-dimensional effects are important. This code differs from the core code in that it represents regions which do not have a myriad of internal surfaces but do have irregular boundaries. The downcomer, plenums, and ECCS injection regions are intended to be represented by the code. A two-parameter differential transport model of incompressible turbulence is considered to be sufficiently general and at the same time computationally economical for the turbulent flows of interest for both compressible and incompressible fluids. The two-parameter VARMINT code served as the prototype for both the core and plenum codes and was obtained from the Science Applications Incorporated (SAI) [38]. It appears that progress stopped at the three-dimensional equal velocity, equal temperature (EVET) stage.

Executive Code

The purpose of the executive code is to allow codes to be coupled together quickly and to transfer data from one code to another. This will permit a complete analysis without any manual data conversion, eliminating potential sources of error. This will allow the code system to be interchangeable with other computers in the nuclear industry other than ANC's. The executive code got as far as linking to the EVET code.

ZVUT Code

The purpose of ZVUT (Zero Velocity Unequal Temperature) Code is to develop prototype forms for the energy partition functions which describe the fraction of the heat flux which enters into a phase change process and which causes a change in sensible energy. The code also is used to predict the fraction of each phase at saturation while some of the vapor is superheated and when one phase or the other disappears.

EVET Code

The purpose of the EVET (equal velocity equal temperature) code is to be a test bed for difference and iteration schemes and described a constant area pipe with prescribed pressure or velocity at either end of the pipe. There were several different versions of the EVET code which tested different finite-difference and iteration schemes. Energy is prescribed at either end, but not both. The equations are clearly hyperbolic and can describe fluid velocities up to the speed of sound.

UVET Code

The purpose of the UVET (Unequal Velocity Equal Temperature) code is to be a test bed for the iteration and differences schemes developed in the EVET code and described a constant area pipe with prescribed pressure or velocity at either end of the pipe. Prescribing pressure and mixture energy fixes the volume fraction of each phase at saturation.

ADF Code

The purpose of the steady-state three-phase ADF (Annular Dispersed Flow) code is to check out prototype friction factors and deposition and entrainment rates in annular dispersed flow in a vertical pipe. The three phases treated are a film on the wall with dispersed two-phase flow in the core. The correlations developed are to be used directly in the UVUT code.

SSUVET Code

The purpose of the SSUVET (Steady-State Unequal Velocity Equal Temperature) code is to check prototrypr friction factors for flow regimes other than annular dispersed flow. Evaluation of the prototype correlations is to ascertain that the results are realistic, compare well with experimental data, and that friction factors are continuous across flow regime boundaries.

UVUT Code

The UVUT (Unequal Velocity Unequal Temperature) also called STUBE (Seriated Tube) code structure was the result of combining the UVET and ZVUT codes. It is the highest level of complexity, contains dummy subcodes for all correlations in modular form, and contains all of the ZVUT energy partition functions. The code describes a constant area pipe with pressure prescribed at the inlet and outlet, and phase energies and void fractions prescribed at the inlet, and uses the EVET iteration scheme.

7.5 Investigations into Why the Pressure Kept Going to Zero for Standard Problem 1

The year 1974 would prove to be quite eventful. Dimitri organized a Round Table Discussion titled Modeling of Two Phase Flow for the Fifth International Heat Transfer Conference in Tokyo, Japan, which was to be held in September. Dimitri sent our at least two dozen letters in July 1974 to various luminaries in the area of two-phase flow asking them to participate. Written responses were received from S.L. Soo, S.-I. Pai, George Rudinger, Francis Harlow, the members of the SLOOP code group (Dan Hughes, myself, Glen Mortensen, Chuck Noble, John Ramshaw, Vic Ransom, Charlie, and John Trapp), J.M. Delhaye, Graham Wallis, K. Namatame, and R.L. Panton. Dimitri edited our response [which included a demonstration that an instability believed to be caused by complex characteristics was stabilized by the addition of a term, I believe the bubble growth term given by Eq. (7.3)], as well as the others which appeared in the Proceeding [28]. This Round Table Discussion was probably the spark that ignited the international controversy concerning the imaginary characteristics. It is unfortunate that the full responses were never published. I still have a copy of them. Dimitri sent an invitation to Sir James Lighthill at the University of Cambridge who gave a lecture at IIT and with whom Dimitri briefly discussed imaginary, i.e., complex, characteristics. Sir James' (as Dimitri always refers to him) response was not included in the published discussion. Some of his comments are interesting and worth quoting. "Provisionally I am inclined to stick to the idea that imaginary characteristics should involve instabilities. There is not necessarily anything physically unreasonable in this, since we could be dealing with two-phase mixtures out of thermodynamic equilibrium. Your equations do not seem to include any feature (e.g., nucleation) that would limit the rate of phase change in such a case.'Plasma streaming' instabilities are another pertinent example where analysis of two-phase motions in the past has led to the recognition of instabilities." Sir James concludes his letter with "…I would like to see in detail what you've submitted to JFM." JFM is an acronym for the Journal of Fluid Mechanics to which our paper was submitted in December 1973. Chapter 8 discusses its fate as well as its long journey to publication.

Instabilities in the EVET code which were basically eliminated by identifying stable iteration schemes using Glen Mortensen's STAB code were used in the UVET and UVUT codes. The instabilities observed in these two codes caused by complex characteristics were mitigated by adding terms such as the added mass [1, 5] and so-called bubble growth terms to reduce the regions of complex characteristics. However, the problem which continued to persist for almost 2 years was the problem of the pressure going to zero using the UVUT, i.e., STUBE, code when simulating Standard Problem 1 based on the Edwards and O'Brien experiment [12]. This would prove to be a major factor in unraveling the LOOP code schedule and contribute to the SLOOP code project's eventual demise. But as we will see shortly, the politics of science ultimately finished the job. The simulation of Standard Problem 1 was shaken down using the test-bed EVET code [39]. Refinement of the boundary conditions at the pipe inlet and exit were formulated to account for prescribed velocity at the inlet and outflow and flow reversal at the outlet.

Figure 7.3 illustrates what was happening near the closed end of the pipe during the depressurization. What should happen is that the pressure decreases until the saturation pressure is reached. Then phase change, or flashing, occurs, and then the pressure levels off. Contrary to this, the pressure continued to decrease until it fell to zero as shown in Fig. 7.3a and then the code terminated when a check for negative pressure was sensed. The volume fraction of steam produced is shown in Fig. 7.3b compared with the EVET code results. The mysterious thing was that away from the closed end, pressure saturations were achieved. It should be noted that without phase change, the wave form at the closed end would reverse. For example, if the initial pressure in a closed inlet pipe was say 10,000 Pa and the pressure at the exit was reduced to an ambient pressure of 9000 Pa, a 1000 Pa drop, the pressure at the closed end would initially fall to roughly 10,000 − 2000 Pa = 8000 Pa and move back to the exit and produce flow reversal. The wave would then reflect off of the exit and move back toward the closed end. As time goes on, waves would move back and forth throughout the pipe until the pressure falls to 9000 Pa at steady state. A test was performed whereby the pressure at the exit was dropped slightly so that no flashing occurred in the pipe including at the closed end. The expected behavior was achieved as just explained. Similar wave behavior was observed in the simulation of the Miyazaki et al. air-water experiment [32]. Another test was performed where the initial temperature was adjusted so that a small pressure drop would cause flashing to occur. No problem was observed at the closed end.

This phase change problem was screened from the sponsor as long as possible. As mentioned earlier, for over 2 years, the SLOOP code pretty well functioned autonomously with negligible if any feedback and oversight from Jerry Griffith the AEC sponsor, with no external review meetings. In spite of this, some of the structure of the advanced code was falling into place. The monthly management reports continued to be vague and did not discuss the UVUT flashing problem for Standard Problem 1. They did include the continuing saga about the complex characteristics and investigations of numerical finite-difference and iteration schemes. All this was about to change.

Now, the politics of science rears its ugly head and starts to work overtime. Larry Ybarrondo informed Charlie early in 1974 that Tong was going to work for the AEC. Because of the circumstances related to Charlie's leaving Westinghouse in 1970 because of Tong's mismanagement and dishonesty, documented in his letter that went all the way to upper management, Tong harbored a great deal of animosity toward Charlie ever since then. Charlie knew Herbert Kouts, Director of the AEC's Division of RSR, from the time he worked as a consultant for the ACRS. Kouts was a member. Charlie telephoned to warn him that hiring Tong would create a conflict of interest. Subsequently, Larry and Charlie went to see Kouts when they were on a trip to Washington. Kouts said Tong was an expert in two-phase flow and heat transfer, and he needed him to guide the two-phase flow development research for the AEC. Then, Larry and Charlie went to a Washington Post reporter to tell him that the fox was being put in charge of the hen house. They informed Kouts that this appointment would be viewed by the public and the nuclear community as an outright conflict of interest. In addition, Charlie told the reporter that Tong was unethical since he had used his reputation at Westinghouse to get his CHF correlations accepted to justify the power levels at which their reactors could run. This was discussed at some length in Chap. 4. It should be noted that at this time Westinghouse was the world's largest supplier of nuclear steam supply systems [40]. Now Tong was going to the AEC and would safeguard those correlations so that Westinghouse would have little problem justifying its operating nuclear plant power levels and thus giving them unfair advantage over its major competitor, General Electric. The reporter replied that this sort of thing happens every day in Washington; personnel switch back and forth from being regulated to being regulators. Tong would then be put in charge of monitoring the advanced code work at ANC. Unfortunately, Kouts informed Tong that Larry and Charlie had tried to stop him from hiring him. Charlie was afraid that Tong would begin a vendetta to kill his SLOOP code project. It would appear that not only was Charlie worried, but Ken Moore was also concerned. He left ANC in January 1974 around the time that the news of Tong joining the AEC was circulating and left for Energy Incorporated to develop RETRAN for EPRI. Ken was section leader of the System Model Optimization Section in which was developing RELAP4 which would replace RELAP3. ANC upper management was concerned that this work would go to Battelle Columbus.

I don't know the exact date, but Tong, and Stan Fabic did leave Westinghouse and joined the AEC early in 1974. Then, shortly thereafter Charlie stepped down as Manager of the Analytical Model Development Branch around February 1974 and then Vic Ransom replaced him. Charlie had this plan in his mind for quite a while. There is an entry in Vic's Record notebook dated January 14 referring to requests to ANC from Stan Fabic which helps to pin down the date. Westinghouse was having deep financial problems with reneging on contracts for uranium yellowcake which it was providing its customers [40], and so it might have been a good time for both of them to leave. Dimitri related to me that Tong had been demoted because of the letters written by Charlie, and perhaps Dick Farman, when they left Westinghouse in 1970 as discussed in Chap. 4. So, this was a good reason for Charlie to get out of the limelight. Tong wouldn't have had any reason to dislike Vic with him as Manager.

With the hiring of Tong to became Assistant Director for Water RSR, his hiring Stan Fabic to become Chief of the Analytical Development Branch and Novak Zuber to become Stan's assistant as Chairman of the Advanced Code Review Group, scrutiny and oversight over of ANC's advanced code effort increased rather quickly. Dimitri related to me that Novak Zuber left Georgia Tech under a cloud that Dimitri says was related to unethical conduct involving financial dealings in the Mechanical Engineering department to get contracts. Therefore, we now had the unhealthy situation whereby two apparently unethical persons were in power over the safety of US nuclear reactors. The LOOP code schedule continued to slip, and the problem would soon become all too evident. Tong bided his time for a while and didn't attack Charlie as soon as he joined the AEC. He hired Stan Fabic to begin the process.

Stan Fabic rather than Tong became the front man interfacing with Vic and his boss Pete Lang Manager of the TRSP since his name started to appear frequently in Vic's Record notebook. Stan who was Advisory Engineer of Methods Development at Westinghouse was a good friend of Charlie's when they both worked together. Charlie thought a great deal of him. When Fabic first started at the AEC and saw what was going on in the SLOOP code effort Charlie remembers that Fabic was ecstatic. Charlie related to me that he didn't know what Tong did to him, but it must have been awful. Overnight, Fabic started attacking the LOOP code project. Charlie recalls … "I'm sure Tong told him if he didn't do so, he would never have another job." According to Vic's Record notebook, on March 25, 1974, Stan announced that there would be a total review of the SLOOP code probably in May. This would turn out to be the fist such meeting since the project began in 1972. By May, information began to leak out that the AEC was going to undergo a reorganization which would create a lot of turmoil and potential funding problems. At about this time, LASL and in particular Group T-3's Harlow who would step down and be replaced by Tony Hirt began entering the picture as Fabic interfaced with them about the characteristics controversy and possibly have them begin work on developing a code to replace SLOOP at ANC. Fabic told Pete Lang that monies for the SLOOP code would be withheld and would then be split between LASL and ANC. The decision on how to split the monies ($450,000) would be come after Fabic visited LASL, an in-house review was to be made by RSR, and a proposed meeting between ANC and LASL and other experts would take place. Fabic was beginning to openly complain that the SLOOP code had no credibility for producing results. News of this filtered into the SLOOP code personnel which began to demoralize them. During the period leading up to the proposed SLOOP code review meeting, there were frequent discussions between Vic and Stan and probably a visit by Zuber to ANC. On July 25, Vic's Record notebook has an entry describing a staff meeting with Pete Lang which is extremely damaging. It states that Fabic thought that the advanced code effort was "…all screwed up—RELAP is full of errors and verification hasn't produced a report worth anything."

This review meeting announced in March for May finally came about all day on June 28, 1974, in Germantown and was called the advanced code (SLOOP) status review meeting. Apparently, there was an earlier SLOOP code review meeting held in Germantown on April 4 at which it was decided what ANC was expected to show results at the June 28 meeting to illustrate the status at the end of ANC's fiscal year (FY 1974) on June 30. By the time of the June 28 review meeting, Bill Yuill, who had been responsible for correlation development for the SLOOP code, was leaving ANC and going to Allied Signal. Ken Moore had preceded him. As I remember, Bill was going to be working on a proprietary process to produce titanium dioxide, TiO_2, which is used in a variety of chemical processes. The review meeting covered the SLOOP code, model development experiments, and the SCORE, SPLEN , and executive codes. I did not attend this meeting. I only have copies of the information shown for the SLOOP code review more than likely made by Vic Ransom. The entry in Vic's Record notebook for June 28 begins with an entry clearly by Charlie, probably because Vic was making the first presentation.

Attendees at this meeting were Pete Lang, Vic Ransom and Charlie from ANC, Charles Gilmore from Idaho Operations, Zoltan Rosztocy and D.E. Solberg from AEC Regulatory, and L.S. Tong, Novak Zuber, Lou Shotkin, and Stan Fabic from AEC RSR. The review apparently began with an overview of the equation development with allusions to the characteristics. To me, it was confusing and was most assuredly so by the RSR personnel. There was discussion of a two-pressure model with addition of the so-called bubble growth term, and the artificial viscosity model. Next, results for Standard Problem 1 from the STUBE code were shown followed by results for steady-state heat transfer from the SSUVUT code, Standard Problem 1 from the EVET code, comparison with Fauske's ANL critical flow pressure data (see Sect. 6.1 in reference [4]) from the UVUT code, and redistribution in a vertical pipe from the UVET code. In the afternoon, there was a presentation by Stan Fabic concerning long range planning whereby RELAP4 would transform into RELAP5 by the end of 1976! In a May 8 letter from Tong sent to the Manager of the AEC Idaho Falls Operations Office before this meeting and passed on to Vic, he mentions using RELAP5 as an intermediate step between the existing, i.e., RELAP4 and the advanced system code. This is the earliest recorded mention of RELAP5. Ominously, he also states that some of the advanced code modules will be developed elsewhere.

In the review of this meeting sent by Tong on July 2, 1974, to R. Glen Bradley, Manager of Idaho Operations Office, eight action items were requested. Item 3 addressed the term ANC called the "…interphase force term coefficient…" which "…does not have a physical basis in a two component code such as UVUT. RSR questioned the logic of using terms that cannot be defined physically just to make the equations solvable." Item 4 addressed the large difference between the steam and water velocities after phase change initiated. It was noted that with the velocity difference calculated, the steam bubble diameter would have to be 10^{-7} cm in diameter and therefore "…the steam velocity as calculated…is considered to be unrealistic." Vic assigned Charlie the task of having the responsible members of his group, including Dan Hughes, Jim McFadden, and myself respond to Tong's review. It took until July 24 for Lang to write a letter to Paul Litteneker, Acting Director of the AEC Program Analysis and Evaluation Division in Idaho Falls, containing ANC's response to Tong's review.

On July 25, Fabic submitted *his* review of the June 28 meeting in a letter to Tong with copies to the attendees (Kouts, Vic Stello, and Stephen Hanauer, Advisor to the AEC's Director of Regulations). It was much more detailed and was heavily negatively critical of ANC's performance. He reviewed the April 4 SLOOP code meeting demands which were to be addressed at the June 28 meeting. They were supposed to be "…results of SLOOP predictions with test data pertaining to some realistic, meaningful problems…to obtain a realistic assessment of the code status" which "…could not be made on the basis of ANC reports which deal with generalities and which confuse the picture by referring to what the code should be able to do rather than what it can do." He went on state that the SLOOP code data comparisons "…would provide RSR with a reasonable yardstick to assess the credibility of ANC's milestones…which promise…" (i) by the end of September

1974 to model the Trojan PWR and (ii) by the end of October 1974 to run Standard Problem 2 [41]. He then started to tear apart the presentations which were made for the conservations equations and comparisons with test data. What he was setting up was an argument which he was about to expound that ANC failed miserably to meet his request.

Of particular concern and impact to me personally were Fabic's critique of the data comparisons I prepared for the meeting. First was the comparison with the critical flow pressure data of Fauske. Although Fabic found the comparison to be reasonable, he thought that any homogeneous thermal equilibrium code such as RELAP could do as well. Then, Stan ripped into the UVUT comparison for Standard Problem 1.

Second on Fabic's list was the criticism of the UVUT comparison with Standard Problem It was at this meeting that Fig. 7.3a was shown and which Stan savagely ripped into as he should have. I myself would have never shown such a negative result. But that's all we had. The code was blowing up, and we had no real explanation why. A weak explanation put forward was that the interface mass transfer correlation was inadequate, yielding insufficient vapor generation to cause repressurization. One of Fabic's recommendations was to have ANC consult with LASL's T-3 and T-7 groups about the conservation equations. He stated that LASL had *already* been asked by RSR to help ANC. Fabic and Lou Shotkin visited Tony (then Group T-3 leader) for two days in 1974 to discuss starting work on water reactor safety. In a telephone conversation with Tony in 2016, he said that he declined to work on an "engineering" code. He did agree to work on several contracts for development of new methods and/or specialized codes for particular applications and suggested Fabic also contact the T-1 group. Work then started with the formation of the R then Q Division working on the TRAC code.

He recommended that such a meeting should be held at LASL toward the end of August since a number of well-known experts in numerical analysis spend their summers there. The second recommendation was that ANC should vigorously pursue the SLOOP description of a PWR with all of the logistics including junctions of unequal area, multiple branches, nodalization of a PWR system, description of a double-ended break, ECC injection, pumps. In reality, none of these tasks had even been started, and to do this by the end of September would have been impossible. To model Standard Problem 2 which was based on the 1-1/2 Loop Semiscale Isothermal Test 1011 described in reference [41] would not be any easier. The SLOOP code continued to flounder after this meeting because of the characteristics impasse and the zero-pressure problem for Standard Problem 1.

Charlie wrote a long letter responding to Fabic's scathing review, but I don't have any evidence that it was ever sent to Fabic or Tong. In my opinion, the proverbial handwriting was on the wall. As reasonable persons, Vic and Charlie were probably shaken to their boots by such a review, but did not show it. They must have known modeling a PWR, or Standard Problem 2, would be impossible. Pete Lang should have jumped all over them, but he was such a nice man and didn't. At least, the project wasn't canceled. I believe that it was this meeting which started the SLOOP code members to start thinking about bailing out.

7.6 The Los Alamos/Aerojet Meeting of August 27, 1974

Because of the above review meetings, we were made aware that the Group T-3 headed by Tony Hirt (Frank Harlow was Group Leader until 1973) were insisting that the UVUT PDE's had to possess imaginary characteristics and therefore there was no problem. ANC kept insisting that there could not be imaginary characteristics because no globally stable finite-difference numerical scheme could be found —the PDE's were ill-posed as an initial value problem. It was at this point that the characteristics controversy really came to a climax. The discussions and arguments flew back and forth among the Group T-3, RSR, and our group concerning the implications of the imaginary characteristics grew intense as evidenced by the two SLOOP code reviews by RSR discussed above. The SLOOP code personnel were beginning to get feedback from RSR through the vine, rumors and maybe Vic and Charlie that in no uncertain terms RSR felt that LASL's Group T-3 had the experts in code development and that the ANC personnel had little credible expertise and maybe had no business doing complex code development. They looked at us like we were a bunch of cowboys. Tong insisted that a face-to-face meeting between ANC and LASL had to be held at LASL to resolve the controversy. This trip to LASL finally took place on August 27, 1974. Representing ANC were Pete Lang, Manager of the Thermal Reactor Safety Program, Vic, Charlie, Dan Hughes, Glen Mortensen, and myself. About a dozen LASL personnel were in the meeting listed below. The legendary Professor Peter Lax from the Courant Institute was also present. No RSR representatives were present. ANC gave a summary of the material prepared for Dimitri's Round Table Discussion. Because of preparations for this meeting, and its timing, no SLOOP code personnel went to the Fifth International Heat Transfer Conference in Tokyo. Frank Kulacki who did his MS under Dimitri at IGT in 1966 read our responses at the Round Table Discussion in Tokyo [28].

This historic meeting was documented in a trip report by R.J. Schultz, ANC Manager of Reactor Behavior Program in a letter to P.E. Litteneker, Acting Director of the Program Analysis and Evaluation Division, Idaho Operations Office of the AEC. It is included below in its entirety and was created from a scan of the original document and converted into Word. The typography adheres as closely as possible to the original.

Aerojet Nuclear Company
550 SECOND STREET
IDAHO FALLS, IDAHO 43401
September 13, 1974

P. E. Litteneker, Acting Director
Program Analysis and Evaluation Division
Idaho Operations Office
US Atomic Energy Commission
Idaho Falls, Idaho

TRIP REPORT—ANC CONSULTATION
WITH LASL ON SLOOP CODE DEVELOPMENT—Scz-29-74
A meeting for interchange of technical information on development of two-phase flow fluid dynamic models and solution techniques was held at LASL on August 27, 1974.

The attendees included the following persons:

Aerojet Nuclear Co.	LASL
P.M. Lang	F.H. Harlow
V.H. Ransom	C.W. Hirt
C.W. Solbrig	A.A. Amsden
E.D. Hughes	T.D. Butler
R.W. Lyczkowski	P.Lax (Courant Institute)
G.A. Mortensen	B.B. Wendroff
	M.M. Klein
	B.R. Suydam
	W.C. Rivard
	J.R. Travis
	S. Orszag (MIT)
	(possibly others)

The meeting was opened by ANC giving a summary of the material which was submitted to the Round Table Discussion, Fifth International Heat Transfer Conference, Tokyo, Japan, September 1974. At the conclusion of this summary, F. H. Harlow stated that: other than for some semantics problems, there exists a surprising state of agreement. LASL personnel did express the opinion that the addition of the $\partial\alpha/\partial x$ term has a stabilizing effect, but without a physical basis. However, LASL adds artificial damping terms to the numerical scheme in order to stabilize high-frequency solution components (wavelengths of order Δx)

bcc: P.M. Lang
V.H. Ransom
R.J. Schultz—2

P.E. Litteneker
Scz-29-74
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also without a physical basis. The semantics problem came about because LASL used the term characteristics to mean the eigenvalues of the dispersion matrix as opposed to the mathematical definition of characteristic roots and surfaces for a differential operator. The remainder of the meeting consisted of a technical discussion on the subject of hyperbolicity, well-posedness, and numerical techniques. Several general conclusions resulted from this portion of the meeting: (1) Hyperbolicity of a differential operator is a necessary condition for a well-posed initial value problem; (2) the initial value problem should be well-posed; (3) the numerical solution scheme must damp components of the solution having wavelengths of order Δx; and (4) it is preferable that the necessary damping in the numerical scheme result from a physically based differential system.

In general, the meeting took place in an atmosphere of openness and cooperation. ANC was very encouraged to find agreement on basic principles for formulating the problem. Even though ANC and LASL's approaches are different in mechanism, they both accomplish the same objective, a well-posed difference problem.

A summary of the technical discussion is attached. No statements are necessarily verbatim, but were reconstructed from notes.

Original Signed by

R.J. Schultz, Manager
Reactor Behavior 'Program

VHR:ds

Attachments - #1 LASL Trip Report
#2 Comments for Round
Table Discussion

cc: H.J. Kouts, RSR
L.S. Tong, RSR
S. Fabic, RSR
S.H. Hanauer, L
V. Stello, L
D.F. Ross, L
L.H. Sullivan, L
T.D. Butler, LASL
G.K. Leeper, ANC
F.H. Tingey, ANC
Attendees

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LASL TRIP REPORT

The initial portion of the meeting consisted of Dr. Ransom of ANC describing ANC's position on the basic equations. This opinion is attached. Basically he stated that the equation set must be well-posed. Most two-phase flow basic equation sets appearing in the literature are ill-posed when dissipation is not included. Dr. Harlow of LASL stated that the basic equations (without dissipation) can only be solved by adding dissipation terns. Since ANC agrees that the basic set of equations can be made well-posed if sufficiently large dissipation terns are added, everyone at the meeting agreed that the ANC and LASL positions coincide. The agreed position was summarized as the following: (1) The basic equation set cannot be solved as is and (2) either the equation set must be improved to include more physical terms in it (e.g., "added" mass, bubble growth, two pressures, transverse momentum) to make it well-posed or terms must be added to the equations even though these terms may be non-physical (e.g., pseudo-viscosity, pseudo-surface tension). This latter point was characterized by Dr. Harlow as being equivalent in the LASL and ANC approaches. That is, ANC has employed analytical and numerical tools to investigate well-posedness and stability of various models of both the differential and difference equations, prior to programming the solution scheme, whereas LASL has programmed the ill-posed equations and will add a pseudo-viscosity term to the finite-difference equations via numerical experimentation. The magnitude of the pseudo-viscosity may have to be much higher than any physical value of viscosity. Thus, in both approaches, elimination of numerical instabilities is the objective and both approaches may lead to introduction of non-physical terms.

Dr. Peter Lax of the Courant Institute said he felt uneasy with these approaches. He thought that in order to have a satisfactory set of equations, they should be well-posed without adding any non-physical terms. He did state that he thought that the ANC and LASL approaches were equivalent.

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Scz-29-74
Attachment 1, page 2 of 3

Several points were raised with respect to the hyperbolicity of initial, boundary value problems. Dr. Lax asserted that such problems are ill-posed if the characteristics of the first-order, quasi-linear differential equations are not real. He further stated that complex characteristics probably indicate that something is wrong with the equations.

Dr. Lax suggested that the equation system should pass the "high-frequency" test. That is, the equations and numerical scheme should not allow small wavelengths to grow. This is a more stringent requirement than the hyperbolicity since it guarantees that the initial value problem is well posed and, in addition, that the system of equations be hyperbolic.

The apparent misunderstanding between ANC and LASL which existed prior to this meeting was a problem of semantics. It became clear that ANC had been discussing characteristics, while LASL had been discussing dispersion relations. Clarification of the use of characteristics also lead to discussion of the implication of characteristics with regard to boundary information, solution-schemes and signal propagation as ANC has been employing them. Since LASL had not considered characteristics, they were not familiar with the implications of complex characteristics in these areas. Dr. Harlow requested that Dr. Lax instruct him on the importance and consequences of characteristic analyses. Dr. Lax agreed to do so. LASL had not considered the question of well-posedness in the differential sense. Their remarks had instead been directed to consideration of possible physical instabilities via use of the numerical dispersion relationship. ANC agrees with their position that physical instabilities of sufficiently long wavelength can exist and should be allowed to exist in the solution. ANC agrees that it is possible and satisfactory to have a complex root of the dispersion equation.

The discussion then turned to a consideration of where Los Alamos might help Aerojet Nuclear in resolving some of the difficulties that Aerojet has encountered in running the SLOOP code. The Los Alamos personnel, in general, stated that they had not progressed to the point that Aerojet was at and consequently they were not

P.E. Litteneker
Scz-29-74
Attachment 1, page 3 of 3

able to offer assistance to Aerojet. They had not, for example, considered how they would be able to describe subcooled boiling. Dr. Harlow stated it would require a significant amount of time before Los Alamos would have a comparable amount of experience to that which Aerojet Nuclear has accumulated in running a myriad of two-phase flow problems with the SLOOP code.

LASL stated that they thought it would be very useful for someone to make up a list of standard problems which should be solved and standard experiments (of the model development type) which should be predicted by both Los Alamos and Aerojet Nuclear to test the SLOOP and KACHINA codes.

Aerojet Nuclear acknowledges the considerable amount of experience LASL has accumulated in solving fluid flow problems. This experience has been incorporated into the fluid flow portion of the SLOOP code. ANC hopes that scientific cooperation will be fostered between ANC and LASL. All present agreed that it was unfortunate that an RSR representative could not have been present.

Most of Attachment #2 appeared in Gidaspow's Roundtable Discusssion [28].

In summary, the major conclusion was that there was a semantic problem which arose because LASL uses the term characteristics in the dispersive matrix of the PDE's as opposed to those resulting from MOC analysis. LASL stated "…that they had not progressed to the point that Aerojet was at and consequently they were not able to offer assistance…" So LASL admitted that the imaginary characteristics were a problem, but no RSR representative was there to hear it. And they never again admitted that after the meeting in their publications and they continued to get RSR funding. As described in Chap. 5, the LASL report for the KACHINA code, which describes the implicit multifield (IMF) numerical technique for multiphase flow, came out in December 1974 followed by three publications in 1974 and 1975. The KACHINA code was never released to the public. See Sect. 5.1 for more details.

RSR subsequently requested that all of the unpublished SLOOP code reports and working notes, bound in large loose-leaf notebooks, be sent to LASL. This struck the SLOOP code group as being highly unethical. Then, on September 21, 1974, Carl Hocevar submitted his resignation, the second to leave the SLOOP code development group, Bill Yuill being the first. Carl then joined the Union of Concerned Scientists. His bitter letter of resignation is included as Appendix G.

The AEC was officially abolished on January 19, 1975, and was reorganized as the Energy Research and Development Administration (ERDA). The regulatory portion of the AEC became a new organization, the Nuclear Regulatory Commission (NRC). This reorganization probably created a lot of turmoil as expected by ANC, and may have helped to keep the SLOOP code from being axed. Therefore, the SLOOP code somehow lurched forward, but its members were becoming demoralized. There were more NRC review meetings, two in January, one at ANC, and another in Germantown, and then the so-called First Semiannual Code Development Workshop held March 17–19, 1975 in Idaho Falls organized by Fabic. As I remember, the first Energy Secretary James Schlesinger attended the Idaho Falls meeting. In my mind, it seems that the real purpose of these meetings was to get the NRC up to date on all the computer code efforts going on at the national laboratories including LASL, Pacific Northwest Laboratory (PNL), and Brookhaven National Laboratory (BNL), such as TRAC, COBRA, and THOR. This was the first review of the TRAC code that I am aware of. The group developing TRAC at LASL broke away from Tony Hirt's Group T-3 in the new Q Division and used some of Group T-3's codes as a prototype for TRAC. The presentation for the SLOOP code was skimpy with no results shown for the UVUT simulation of Standard Problem 1. The STUBE code was still blowing up with the zero-pressure problem.

After the First Semiannual Code Development Workshop in March, I set my mind to get to the root cause of the problem with the pressure going to zero at the closed end during the calculation of Standard Problem 1 with the STUBE code. I don't know what inspired me. It may have been the ZVUT code which had a plethora of models for mass transfer [42]. I started from first principles starting with the mixture energy equation expressed in entropy form, used some basic thermodynamic relationships, assumed thermodynamic equilibrium, and then used the chain rule to convert entropy derivatives to pressure derivatives to derive an expression for the rate of mass transfer due to pressure changes known as flashing. This derivation appeared in an obscure conference paper in 1977 [43]. The derivation per se was never submitted to a peer-reviewed journal. It was extended to three dimensions and used much later to analyze a liquid-sodium fast breeder nuclear reactor experiment using the BACCHUS-3D/TP code [44]. I was able to convince Glen Mortensen to program this flashing expression into the STUBE code. He thought that it just might work after his many failures to find a solution. Dan Hughes says that it was he who submitted the updated STUBE code to run Standard Problem 1. He dropped off the card deck (yes *cards*) at the computer science center in the evening, and the next day the output was on the output counter. Lo and behold, Standard Problem 1 had run to completion for the very first time! The problem was that the phase change was not updated soon enough in the iteration scheme. The solution was to incorporate the flashing model directly into the matrix which solved the pressure equation in the fully implicit solution scheme. All of the impenetrable models that were developed in the ZVUT code (and which for the like of me, nor anyone else, could truly understand) were turned off. The news was reported to Vic who passed it on to Pete Lang who said "This changes everything." However, it was too little, and far too late. Somebody had the idea of submitting news of this accomplishment to both the Idaho Falls Post Register and the Idaho National Engineering Laboratory News. (The NRTS was renamed the Idaho National Engineering Laboratory (INEL) in August 1974.) The May 20, 1975, issue of the Post Register contained the article "LOOP code project marks key advance." The June 4, 1975, issue of the INEL News contained a front page picture of Charlie, Glen Mortensen, Jim McFadden, Bob Narum, Chuck Nobel and myself huddled over a table over the caption "Code Project Team Achieves Major Goal." A scan of this photograph is shown in Fig. 7.4. In my opinion, this was all a sham meant to feed ANC upper management and perhaps lift the SLOOP code participants' morale. It didn't work. In fact it was at about this time Charlie had left the SLOOP code effort entirely to become a Branch Manager of the LOFT Program Division. It was Charlie's hope that Tong would then leave the SLOOP code program alone. It didn't work.

On April 28, 1975, Vic wrote an interoffice correspondence to C.F. Obenchain at ANC Headquarters sending what he called a preliminary report documenting the analysis of Standard Problem 1 using the STUBE code [45]. The report was signed by all of the individuals who had suffered over the last couple of years trying to run this simulation: Chuck Noble, Bob Narum, Jim McFedden, Charlie Solbrig Glen Mortensen, Dan Hughes, and yours truly. It included as an appendix my derivation of the flashing model that saved the day. It is basically the same as the publication in the 1977 Thermal Reactor Safety Conference [43]. On June 5, 1975, Vic wrote another interoffice correspondence, this time to J.H. Ramsthaler (why the change of addressees is a mystery to me) at ANC headquarters submitting what he titled his First Quarter Technical Progress Report [46]. This 54 page document was more than likely intended as a contribution to ANC formal quarterly reports which started for January–March 1975. Contained in this report was progress reported for the LOOP, SCORE , and executive codes. One of the longest sections on pages 21–35 was the reporting for the STUBE code results analyzing Standard Problem 1 which had just been reported as having been successfully performed [46]. This material never appeared in any subsequent ANC quarterly reports. The STUBE code analysis was

(a)

Dr. Solbrig, standing, discusses LOOP Code development plans with, from left to right: Chuck Noble, Dr. James McFadden, Dr. Glen Mortensen, Robert Narum and Dr. Robert Lyczkowski.

(b)

Code Project Team Achieves Major Goal

A major advancement in the science of nuclear reactor safety analysis has been achieved by personnel of Aerojet Nuclear Company's Advanced LOOP Code Project, according to Dr. P. M. Lang, Manager of the Systems Safety Research Division.

Describing this development, Dr. Lang said an advanced analytical model, or computer code, has been applied successfully to a standard steam-water flow problem which encounters some of the fluid behavior which would occur during accidents in high pressure water systems and (postulated for risk assessment purposes) in nuclear power plants. The model has been under development at the Energy Research and Development Administration's Idaho National Engineering Laboratory (INEL) for about three years.

The ANC project is part of a program to develop more accurate models of steam-water flow processes for use in reactor design and safety assessment that is being sponsored by the Nuclear Regulatory Commission (NRC) Office of Nuclear Regulatory Research.

Development of this code has entailed research to define: the basic hydrodynamic model; methods for incorporating physical data; numerical methods for solutions of the system equations; and advanced computer coding techniques for application to scientific computers.

Contributors to this ANC research project are Dr. Daniel Hughes, Dr. Robert Lyczkowski, Dr. James McFadden, Dr. Glen Mortensen, Robert Narum, Charles Noble, Dr. Charles Solbrig and William Suitt.

The application of the Advanced LOOP Code to a standard flow problem was described by Dr. Solbrig, project leader, at a Code Development Workshop, sponsored by the NRC recently in Idaho Falls.

(Continued on Page 4)

(c) (Continued from Page 1)

Dr. Solbrig has been associated with water reactor safety research for the past several years and is a consultant to NRC's Advisory Committee on Reactor Safeguards.

Other Energy Research and Development Administration (ERDA) contractors who are helping to develop system or component models include Los Alamos Scientific Laboratories, Battelle Northwest Laboratory, Brookhaven National Laboratory and Argonne National Laboratory-East.

Fig. 7.4 (**a**) SLOOP code project team. (**b**) Code project team article page 1. (**c**) Code project team article page 2. Source: INEL News, June 4, 1975 subsequently published in another relatively obscure conference proceedings, and so its impact became hidden from future investigators in the nuclear reactor safety community [47]. This publication contains the finite-difference implementation of the flashing model into the pressure equation matrix.

The Advanced Code Review Group Meeting was held June 11–12, 1975, in Germantown which Zuber organized. Once again code developers from LASL, PNL, and BNL came to present progress for code development including the SOLA-DF, SOLA-TIF, COBRA, and THOR computer codes. A host of consultants were invited to the meeting constituting a veritable all-star list of luminaries including Peter Lax, Clifford Truesdell, Garrett Birkoff, and Peter Griffith. The results comparing STUBE code results for Standard Problem 1 were presented. The review of the SLOOP code results were as highly negatively critical as for the Advanced Code (SLOOP) status review meeting held June 28, 1974. Some of the comments contained in Zuber's minutes of this meeting dated July 7 sent to Kouts and other in high command in the NRC are as follows. "Although SLOOP is an advanced code, the predicted results show no better agreement with experimental data than predictions made by simpler codes presently available, for example, by RELAP." This echoes the RSR criticism of the comparison with critical flow pressure data of Fauske from the UVUT code in 1974. "Unrealistically high vapor velocities and slip ratios were predicted. These excessively high values could have resulted from the use of Baker's steady-state map [48] to determine flow regimes during blowdown transients." This echoes the RSR criticism of the comparison with Standard Problem 1 using UVUT in 1974. "By letting the factors F_{gs} and F_{ls} (which account for the effect of thermal non-equilibrium) to be equal to unity, the assumption of thermal equilibrium was introduced in the computations." The criticisms of the other computer codes results by BNL for the THOR code, LASL for the SOLA-DF and SOLA-TIF codes, and by PNL for the COBRA code were quite benign.

7.7 SLOOP Code Development Implodes Scattering Most of the Participants

Such negative criticism served to brake the camel's back for the SLOOP code. In spite of all the effort expended on resolving the zero-pressure problem for the analysis of Standard Problem 1, it was not enough. After this Advanced Code Review Group Meeting which I did not at attend, resignations from the SLOOP code began. Dan Hughes and Jim McFadden left for Energy Incorporated and Glen Mortensen left for Intermountain Technologies, Inc., founded by George Brockett, both companies located across town in Idaho Falls. John Ramshaw left for LASL to join Tony Hirt's Group T-3. This was probably sparked by Dan Hughes' feedback from this meeting. He remembers that during his presentation for the SCORE code as he showed the slide for the volume averaged equations being solved and he said

"We solve the three-dimensional Navier-Stokes equations." Someone in the audience, Clifford Truesdell if he correctly recalls, said, in a rather loud and threatening voice, "You call those the Navier-Stokes equations!" The criticism of what Dan showed was contained in the minutes of the meeting which questioned the validity of the volume averaging procedure. On June 24, Pete Lang sent a memo to the Analytical Model Branch personnel announcing that "…V.H. Ransom is relinquishing his duties as Manager…in order to be able to devote his full time to technical activities again." Pete assumed the role of Alternative Manager. With Vic stepping down, and Charlie, Dan Hughes, Jim McFadden, and Glen Mortensen gone, there was a noticeable vacuum formed. Charlie stopped keeping track of what was going on except to note that many people left the group and so he didn't don't know the details of how Vic was able to keep any of the remaining group and work going. Vic stayed on as did Chuck Noble and Bob Narum.

I started wondering to myself, maybe I should leave too. So I resigned on July 14 and the next day started employment at Energy Incorporated. The agreement was that no increase in salary would be given so as to eliminate the charge that EI was pirating ANC employees.

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Chapter 8
The Characteristics Paper Caper

I begin this chapter by relating an incident that would play a major role in future relations of Dimitri and myself with Novak Zuber. Before I presented our paper at the ANS Winter in November 1975, Dimitri and I both went to the 14th National Heat Transfer Conference (NHTC) held in Atlanta, Georgia in August, 1973. There we met with a friend of Dimitri's and a former classmate of his while at IIT, George Buzena,, who graduated in 1962 with an M.S. in Mechanical Engineering. Dimitri graduated with his Ph.D. also in 1962. George left IGT and went to Yale University for his Ph.D. He was then a Professor on the faculty of the School of Mechanical Engineering at Georgia Institute of Technology (known colloquially as Georgia Tech) and offered to give us a tour of Novak Zuber's Two-Phase Flow Laboratory, one of the laboratory facilities in the Mechanical Engineering School. George is now Emeritus Professor of Mechanical Engineering from Florida State University at Tallahassee, Florida. This tour scheduled for Tuesday morning November 7 was offered to participants of the NHTC. Zuber had been at Georgia Tech since 1969 after he left the Mechanical Engineering Department at New York University. While we were looking around at the equipment in the laboratory and George was explaining their function as best he could, Zuber came storming in and began ranting and raving in a loud and forceful voice, accusing us of "spying" on him and said he would report us to the AEC. I was terrified as this was my very first contact with him. Dimitri's friend George tried, in his usual mild manner, to do his best to quiet Zuber down. Then Zuber stormed out of the laboratory perhaps going to phone the AEC. Subsequent to this tirade, George, Dimitri, and I left the laboratory quietly. Needless to say, I was totally upset. Maybe the AEC would revoke my "L" level clearance which would cause me to lose my job at ANC. Maybe Dimitri's consulting agreement with Charlie would be canceled. When I returned to Idaho Falls after the meeting, I reported this dreadful incident to ANC management. No correspondence that I know of was ever received from the AEC as Zuber promised he would report Dimitri and me. No disciplinary actions resulted from the ANC or the AEC, and the incident was forgotten, at least by us.

R.W. Lyczkowski, *The History of Multiphase Science and Computational Fluid Dynamics*, Mechanical Engineering Series,
https://doi.org/10.1007/978-3-319-66502-3_8

Zuber's outrageous behavior was legendary. While he was still a professor at Georgia Tech, Charlie witnessed an oral review he gave at an International Heat Transfer Conference for an excellent paper by the then Chair of his department, Professor Stothe P. Kezios. He was an esteemed member of the heat transfer community, former Chair of the Mechanical Engineering Department at IIT, and a good friend of Dimitri. Reporters rather than presenters were common at early International Conferences. They had the opportunity to review presentations and comment on them at the sessions. This practice has, unfortunately, been abandoned. Zuber's review was so deprecating and unfounded that Kezios turned beet red and remained silent. This may have contributed to Zuber's exit from the department at Georgia Tech and his joining the NRC. Recently Dimitri recalled for me another example of Zuber's outrageous public behavior. It occurred in 1975 at the 15th National Heat Transfer Conference in San Francisco, where I presented my paper, "Transient Propagation Behavior of Two-phase Flow Equations" discussed in Sect. 8.2. Either during or after my presentation, this is a paraphrase if not close to what he actually said: "If you knew high-school physics and understood the concept of pressure you wouldn't be putting the pressure in the continuous phase only."

8.1 The Journal of Fluid Mechanics Paper

I mentioned toward the end of Chap. 6 that Dimitri and I wrote a manuscript titled "One-Dimensional Two-Phase Flow Equations and Their Characteristics" which was prepared for the November 1973 American Nuclear Society (ANS) Winter Meeting to be held in San Francisco. However, it was not submitted to the ANS for publication in Nuclear Science and Engineering. This chapter now traces the long tortuous journey that this manuscript undertook on its way to publication in the open literature. It begins when Dimitri and I must have thought the manuscript was important enough to submit it to the prestigious Journal of Fluid Mechanics. On December 14, 1973, I mailed three copies of the manuscript to J. W. Miles, unchanged from the manuscript prepared for our ANS presentation, along with photographs of the figures suitable for publication. On May 13, 1974, we added Appendix B, Homogeneous Equilibrium Model, while the manuscript was still under review. Although I received a postcard acknowledging receipt (as I did for the manuscript itself), I don't think that this appendix was ever sent to the reviewers for consideration. On June 26, 1974 Professor John W. Miles from the University of California, San Diego, sent me four reviews. His cover letter stated: "We have now received reports from four referees (see enclosed) on your paper 'One dimensional two-phase flow equations and their characteristics'. I am afraid that all recommend against publication of the paper, primarily on the grounds that *it is physically unrealistic* [my emphasis]. I am afraid that the reports are sufficiently negative so that I can hold out no hope that a revised version would be acceptable. I am returning your paper herewith. Yours sincerely, John W. Miles Associate Editor Journal of Fluid Mechanics."

I think it worthwhile to include these reviews in their entirety since they demonstrate the reviewers' lack of understanding concerning two-phase flow and the major issues contained in the manuscript: the form of the one-dimensional two-phase momentum equations and the method of characteristics to classify them. These issues are still reverberating to this day. The four reviews are included in Appendix C. I will now comment briefly on some of the more egregious statements. Reviewer A: "This reviewer is unable to find in this paper a rational physical concept justifying the equations for one-dimensional two-phase flow proposed by the authors." Obviously this reviewer is referring to the momentum equations. We didn't "propose" these equations. They were all taken from publications in the open literature to which we gave the references. Reviewer B: "My first objection is that there are no reasons to expect a totally hyperbolic system of equations in practical circumstances. There is no proof or evidence that for a general liquid-gas flow the system of equations should be totally hyperbolic." This statement is a little ambiguous. Clearly this reviewer was unaware of the work of Abbott and Rudinger, referred to in the manuscript, who require their equations be hyperbolic to be able to solve them by MOC. Reviewer C: "Unsteady incompressible flow of a single phase doesn't have real characteristics to my knowledge." This was the most egregious statement made by any of the four viewers and by itself would cause any author to totally discredit the editor of the journal for choosing such an uninformed reviewer. In addition, obviously this reviewer never heard of the vast literature concerning gas dynamics. Reviewer D: 1.) "The proposed formulation assumes implicitly that the two-phase mixture is homogeneous over distances small in comparison with the physical lengths of the problem. For problems of moderate or high condensed volume fractions this is not true. The formulation is valid over a quite restricted range of volume fractions." This reviewer did not understand that the equations are valid over the entire rage of phase volume fractions and not limited to a "restricted range." After this depressing round of reviews, Dimitri and I shelved the manuscript since we were preparing material for his Round Table Discussion Session Modeling of Two Phase Flow at the Fifth International Heat Transfer Conference to be held in Tokyo, Japan in September 1974. There was also the controversy which arose with LASL over the characteristics which the NRC was eager to settle by requesting members of the SLOOP code group journeying to LASL to resolve this issue on August 27, 1974, as described in Chap. 7.

8.2 The 1975 ASME Winter Annual Meeting Paper and Presentation

In early March 1975, I received an announcement and call for papers by mail from Owen Jones in the Reactor Analysis and Safety Division at Argonne National Laboratory in Illinois. It was for the session Fundamentals of Two-Phase Flows to be held at the 1975 ASME Winter Annual Meeting to be held November 30–December 4, in Houston, Texas. The sponsors were the ASME K-8 Standing

Committee on Theory and Fundamental Research and the K-13 Committee on Nucleonic Heat Transfer. The organizers of this session were, Novak Zuber, formerly at Georgia Tech and now at the Nuclear Regulatory Commission, Professor Ralph Powe of Mississippi State University, and Owen Jones. The session would deal with the fundamental nature of two-phase flow from both an experimental and analytical viewpoint. Mentioned in the announcement was the statement that follow-up on work discussed or presented at the Fifth International Heat Transfer Conference held the previous year in Tokyo would be most welcome. This aspect of the session motivated me to consider responding to Owen Jones' flyer.

In lieu of the abstract required, on March 14, 1975, I submitted a manuscript which was by then in two parts. The first part titled "On the Stability of Ill-Posed Partial Differential Equations Part I: An Application to Two Phase Flow" was an expanded version of our response [1] prepared for Dimitri's Round Table Discussion [2]. It included an appendix containing a copy of comments sent to me in a letter on November 27, 1974, by Professor Peter Lax from the Courant Institute of Mathematical Sciences at New York University. These comments pertained to a draft of this manuscript that I promised to send to him during an animated conversation we struck up riding to the airport (in a jeep as I recall) after the historical meeting at LASL we attended on August 27, 1974. The text also contained footnotes which referred to paraphrases of these comments as "Private communication, P. D. Lax." In his letter Professor Lax stated "The notion of characteristics is applicable only to systems which are of the same order in t as in x. A more general notion which is applicable to systems of differential equations of any order is the exponential growth rate when the initial data are oscillatory with frequency ξ. This notion is applicable to 2-phase flow even when you add higher order terms incorporating other physical effects. Of course there is still a linear notion. Instability in the sense of von Neumann is the analogy for difference schemes. It is easy to show and is worth formulating as a general theorem that is that is a differential equation exhibits exponential instability then any difference scheme approximating it fails the von Neumann test for small frequencies. Of course, there is the possibility of instability for high frequencies." "…I think the paper would be a contribution to the engineering literature, but not to the mathematical literature. I am trying to get involved seriously in 2-phase flows."

It is worthwhile to quote extracts of the comments that Professor Lax made for the record. "Real characteristics are necessary for well-posedness but not sufficient. For that one needs a little extra: strict hyperbolicity (distinct characteristics) suffices, but is not necessary. Symmetry is sufficient but so is smooth symmetrizability. Lower order terms can influence well posedness of a FOPDE. For example, the initial value problem is O.K. for

$$1) \quad \begin{aligned} u_t &= 0 \\ v_t &= u_x \end{aligned}$$

but not O.K. for

$$1)' \quad \begin{aligned} u_t &= v \\ v_t &= u_x \end{aligned}$$

The same switch from stability to instability can occur through the addition of lower order terms in difference schemes. …What you call Lax's condition is due to Friedrichs when the C_j [coefficient matrices in a difference scheme] are symmetric matrices. In the unsymmetric case I only showed that this condition implies the von Neumann condition, not stability. It is not true that in most difference schemes the C_j are linear combinations of the A_j; [coefficient matrices $A_j = A^{-1}\widetilde{A}_j$ where A is the coefficient matrix on the temporal derivatives and $\widetilde{A}_j$ is the coefficient matrix on the spatial derivatives] for higher order schemes higher powers of A_j enter; e.g., that is the case for the Lax-Wendroff scheme."

Part II given the new title "Classification of One-Dimensional Two-Phase Flow Equations" was a very slightly modified and reformatted version of the manuscript rejected by Professor Miles in 1974 with the addition of the Appendix B sent to him during the review process. It now contained a table of contents.

Owen Jones responded on April 2, 1975, inviting me to submit a full manuscript for review. Usually, one gets a little postcard acknowledging receipt of such a submission with instructions on how to proceed. In this case, he sent me a letter giving rather explicit instructions on how to revise the manuscript. He stated that

> There was…a considerable amount of discussion of your proposed paper regarding its analytical content. We are pleased to inform you that we would like to obtain a full manuscript from you for review. It was judged, however, that the majority of part 1 was in the nature of a review of material already existing in the literature of mathematical physics rather than a fundamental addition to the body of knowledge. Acceptance of the paper for the review process was decided to be on the basis that the two parts are suitably combined into a single paper having the necessary theorems, etc., which are well known, shortened considerably and included as appendices to the main report rather than in the body of the paper.
>
> If you and your co-authors are willing to make this change in accordance with the attached instructions, we will he happy to have the result refereed for inclusion into the session, and believe it could then be a valuable and interesting addition to the program.

The letter was signed by Owen Jones, Jr. with Novak Zuber's and Ralph R. Powe's names below his. The manuscript instructions stipulated that four copies of the revised manuscript be sent to Professor Powe and one to each of the other session organizers Owen Jones and Novak Zuber and to include the names of three people qualified as referees. The length limitation was 6000 words (24 pages) including figures, each one of which counted as one page.

I worked on a revision which combined these two manuscripts into one. I put the theorems and material pertaining to hyperbolicity in Part I into Appendix A Summary of Mathematical Definitions and Theorems on Hyperbolicity and Well-Posedness. The appendix containing Peter Lax's comments was cut as was an example applying stability analysis to the single-phase potential flow equations at constant energy. The rest of Part I was combined with Part II, and the two Appendices from Part II were placed after Appendix A as Appendices B and C. The combined manuscript was now 57 pages long not counting the Contents page with each figure occupying its own page. The rather long title now read "Characteristics and Stability Analysis of Transient One-Dimensional Two-Phase Equations and Their Finite Difference Approximations." I submitted the requisite copies of the manuscript to the organizers on May 21, 1975. The three people I singled out which I recommended would be qualified to review the manuscript were Jean Boure, George Rudinger and Fred Moody. I received the acknowledgment by letter dated June 2 of Professor Powe's receipt of the manuscript and that as soon as the reviewers' comments were received that he would inform me of his decision regarding it.

A total of *five* reviews were sent me by Professor Powe accompanying a letter dated July 7 which I received on July 14. As I explained in Chap. 7, this was the day I resigned from ANC. The next day I joined Energy Incorporated located in downtown Idaho Falls just across the Snake River from my office in the ANC Computer Science Center. Ralph Powe stated "You will note from these comments that your paper is somewhat controversial. However, due to the currency of the topic the session organizers feel that this material should be made available for examination by the engineering community. In view of the forgoing, we decided to accept your paper provided that you will agree that the presentation time will be available for invited discussion." In a form letter sent by Owen Jones to the authors of the session following up Professor Powe's letter, he highlighted a bullet echoing that the paper had been accepted for presentation and that the reviews were mailed under separate cover. In another highlighted bullet he stated the following. "Although the paper was accepted, the reviewers were somewhat critical regarding one or more areas. …Acceptance of your paper is based on the condition that these criticisms are fully accounted for by suitable revision or a detailed explanation of any differences which exist between your viewpoint and that of the referee." What he did *not* highlight was a bullet forwarding the reviews to the senior editor of the Journal of Heat Transfer for his consideration. He included the manuscript kit and instructions for preparation and typing on the special mats provided from which direct photoreduction copies would be produced (note that this was in the era before word processors and email). He emphasized in bold letters that the mats had to be in his hands no later than July 20 or the paper would automatically excluded from the program.

Of the five reviews, four of the manuscript reviewers I, II, IV, and V recommended acceptable with revision and reviewer III recommended rejection. None of them recommended that the paper be published in ASME Transactions, i.e., the Journal of Heat Transfer. One recommended publication in pamphlet form with a digest in the ASME members' magazine, Mechanical Engineering. These reviewers were generally much more informed then those for the Journal of Fluid Mechanics. The main concern with all five reviewers was the issue of the form of the pressure gradient term. Is the void fraction inside or outside? Except for Reviewer III who recommended rejection, the reviews offered constructive comments on improving the manuscript. Extracts of the five reviews are contained in Appendix D along with extracts of my responses.

Horrors! I had only 5 days to revise the manuscript, type it on the ASME mats supplied and have it arrive from Idaho Falls in Owen Jones' hands at his office in Argonne National Laboratory in Illinois on July 20. I soon realized that it would be impossible to include a major revision to the manuscript and meet this deadline. I must have phoned him to explain the situation and to inform him of my change of employment. In Owen Jones' letter accepting the manuscript described above, he stated that the response to the reviewers' comments could be in a revision or in a detailed discussion. So, I decided to make minimal changes in the manuscript and to prepare a detailed letter describing my responses to the set of five reviewers' comments. This required a four page densely worded letter which was mailed together with the completed mats on July 21, 1975. On July 23 Owen Jones called me requesting that the figures and text should contain SI units. They were added to the figures, and glossy photographs were mailed to him. I also indicated in a copy of the mats where the SI units were to replace the English units. In my letter I requested that our paper be considered for publication in the Journal of Heat Transfer. This was never done. I also sent copies of the papers "Pipe Blowdown Analyses Using Explicit Numerical Schemes" and "Transient Propagation Behavior of Two-phase Flow Equations" which were to be presented at the 15th NHTC in San Francisco, August 10–13 [3, 4] and a "Stability Analysis of RELAP4 with Slip" at the ANS Annual meeting, also located in San Francisco, November 16–21 [5]. It was at the 15th NHTC that I first met J. M. Delhaye from Service des Transferts Thermiques, Centre d'Etudes Nucleares de Grenoble (CENG), France. As I recall, it was at this meeting that members of the code development group from Whiteshell Nuclear Research Establishment, Atomic Energy of Canada, Limited, (lead by Sanjoy Banerjee) with which the SLOOP code group had developed informal but close communications over the years, expressed dismay at its dissolution and wondered what would be the way forward. I couldn't imagine what the way forward could possibly be. What a busy year for me!

I should mention that the publication of the two papers which were presented at the 15th NHTC was held up for 3 years due to the intervention of an individual or individuals from the NRC who had issues with several of the papers presented by authors who from ANC (later EG&G Idaho, Inc.) and Energy Incorporated. They attempted to block their publication. John Chen who was the editor of the Symposium Volume for AIChE papers stuck with it and finally had the volume published. I received a postcard from him dated July 28 indicating that the material had been received with thanks. The paper was not dropped from the session! A letter dated September 2 from the ASME Meetings Administrator in the New York City headquarters office requested my biographical information, technical background, and the names of suggested discussers of the paper. I suggested Owen Jones, George Rudinger, and Fred Moody.

In a letter dated October 24, 1975, Owen Jones sent me two sets of prepared discussions on our paper. One was by Mamoru Ishii from Argonne National

Laboratory and one by J. A. Boure, J. M. Delhaye, and A. J. Latrobe from the Service des Transferts Thermiques, Centre d'Etudes Nucleares de Grenoble (CENG), France. The reason for choosing this particular set of two discussers is now quite clear to me with the passage of time. Mamoru Ishii was a student of Novak Zuber's while at New York University where he began his Ph.D. thesis under his guidance. He completed his Doctoral thesis in 1971 at Georgia Institute of Technology which Zuber joined in 1969. Arthur Bergles was the Chairman of Ishii's thesis committee. After graduating from Georgia Tech, Ishii went to CENG in Grenoble, France as a visiting scientist and worked with Boure and Delhaye. There he published his book on two-phase flow in 1975 [6] which was an outgrowth of his Doctoral thesis. Own Jones is listed in the acknowledgments section of the book, which must have just been published, as carefully reviewing the manuscript. Ishii's book is referred to by Reviewer I of our manuscript. It turns out that Ishii joined ANL and worked with Owen Jones who probably hired him. Jones then left to join Brookhaven National Laboratory (BNL). Ishii is still employed at ANL at the time of this writing. In 1973 Boure, Bergles, and Tong published a review together on two-phase flow instability [7]. Hence there was a clear and close association between Jones, Zuber, Boure, Delhaye, Ishii, Zuber and Tong which constituted yet another aspect of the politics of science theme of this book. Owen Jones must have sent me the call for papers for this ASME session as "bait" to which I (in retrospect perhaps foolishly) responded. Tong, with the help of Zuber, were the ones that designed the eventual destruction of Charlie's SLOOP code effort at ANC as described in Chap. 7.

Owen Jones stated in his carefully worded letter "As you can see, these comments are quite detailed and well thought out, and bear directly on some of the major concerns we have in this particular area. It is our intent that these comments be circulated in a single package along with rebuttal which you might wish to prepare following a verbal presentation of your paper and the discussions at the Winter Annual Meeting. If you wish to include your rebuttal in the package which will be circulated, and it is our desire that you go this if at all possible, please return the copy to me no later than November 15, 1975. The form of the rebuttal should be similar in appearance to the form of each of the written discussions." He then described the format of my rebuttal in detail. He then went on "Please remember that your formal presentation of your paper should take no longer than *5 minutes or so* [my emphasis]. This will leave time for oral presentation of the two enclsed sets of comments, followed by your final rebuttal. After this formal presentation the matter will be thrown open for discussion by all the attendees. It is our wish that we, through this method, will resolve some of the problems which have existed in the areas of multiphase formulation or, failing this, at least point the direction for an eventual solution to the problem." The letter ends with "We look forward to an orderly but fruitful and provocative session and are quite interested in seeing your response to these comments." (I'll bet they were!) For all intents and appearances this was beginning to look like the Inquisition or a Ph.D. final oral examination.

I prepared the written rebuttal with some help from Dimitri and mailed it on November 14. Our paper was published as a formal ASME preprint, and the Discussion was printed separately and distributed to the session participants [8]. An abstract of our paper appeared in Mechanical Engineering [9]. I'm not sure if the Discussion preprint was ever made generally available outside the session by ASME and probably does not constitute a publication. Therefore, scanned copies of Ishii's and Boure et al.'s discussion and a rekeyed version of our rebuttal are contained in Appendix E. As I recall, I made my presentation in 5 minutes flat. To tell the truth I cannot recall the tenor of the carryings on after my presentation. I must have been in some sort of haze. I have retained a copy of Boure's view-graphs used in his discussion. He discussed what constitutes a pure initial value problem. He also showed why both forms of the pressure gradient with the volume fraction inside or outside are acceptable provided that the stress terms are properly accounted for. All in all my impression is and always has been that Boure's papers are quite didactic and fairly impenetrable to the practicing two-phase engineer.

I received several requests for our paper including one from England and one from Japan. Ralph Powe sent me a nice letter dated December 8, 1975, in which he stated "We were very pleased with the results with the results of these sessions and trust that you feel likewise." Owen Jones sent a letter dated December 9 in which he stated "This is just a brief note to express my appreciation and that of my co-chairmen for your cooperation in making the discussion session on your paper a success. I believe that considerable interest was generated in this particular area and that while perhaps no definite conclusions were drawn at the meeting, the net result was to provide some direction for those interested in the field." He included a third formal discussion received too late for inclusion in the Discussion preprint as the discussers could not attend the session. This discussion was by F. J. Moody, B. S. Shiralkar, and J. M. G. Andersen from General Electric Company, San Jose. Fred Moody was one of the discussers I had recommended to Owen Jones. The last author was listed as from the Danish AEC and was probably a visiting scientist or engineer. They thought that "We have concluded that whenever complex characteristics appear from the six-equation model for separated two-phase flow, it indicates that the flow pattern must undergo transition to other flow regimes, e.g., slug, bubble, or homogeneous, for which the governing equations also undergo transition, and real characteristics are obtained." After they briefly summarize the findings of our paper, they state "The main reason that complex characteristics appear in separated flow is that a number of elements which determine flow pattern are missing from the equations, e.g., virtual masses and surface tension." They conclude with "Use of models like the Zuber-Findley void drift model, however, will reduce the number of momentum equations from two to one, in which case it can be shown that the relative phase velocity is less than the velocity of sound of either phase, five real characteristics will always result." Recall that Novak Zuber was employed at the General Electric Company in Schenectady, New York, from 1960 to 1967 when he joined New York University in 1967.

8.3 The Nuclear Science and Engineering Paper

Since as mentioned earlier, the paper was not transmitted to the editor of the ASME Journal of Heat Transfer; it looked like the paper had reached the end of the road and would sink into obscurity. Because I was very busy with projects at Energy Incorporated, a long time elapsed before I got to thinking about trying to get the characteristics paper published in a peer reviewed journal. Since our first publication [10] on the subject was at the 1973 American Nuclear Society Winter Meeting, I decided to try submitting it to the American Nuclear Society publication, Nuclear Science and Engineering. On September 8, 1976, I finally submitted the manuscript to Dixon Callihan, editor of the journal for review. This Manuscript consisted of either a copy or the actual ASME pamphlet 75-WA/HT-23 [8]. In my cover letter I was forthright and wrote "…This manuscript as had a long, rocky road on its way to archival publication because the subject is controversial." I briefly summarized the history of the paper starting with the 1973 ANS meeting and the 1975 ASME meeting. I went on to say "There appears to be no middle ground on the subject. Either critics dismiss the analysis as incorrect or embrace it by using the same techniques themselves. I myself applied the method to analyze "RELAP With Slip" [5] at the 1975 San Francisco meeting of the ANS. I know of several more similar analyses since then. No less than four papers at the recent transient two-phase flow specialists meeting in Toronto refer to the paper. I am proposing to you that a series of two papers be submitted for publication in Nuclear Science and Engineering. They would be the manuscript enclosed with some revisions I have in mind and another manuscript concerning similar analyses on slip versions of the two-fluid model. I doubt that you can find an unbiased reviewer at this stage. I can supply printed comments and rebuttal circulated at the ASME meeting on the enclosed manuscript to prove this point. Please read the manuscript and if the topic appears to be appropriate for your journal, please let me know. Controversial or not, I think the paper deserves an archival publication since it will be referred to more in the future." Wow, did I have a vision! As of June 2017, the paper has had 207 citations on Google Scholar, a thoroughly respectable number. Time went by and no acknowledgment or response was forthcoming, and so on January 18, 1977, I wrote a letter inquiring if the manuscript was received and if it was not, I would resubmit it. About a week later I received an unusual form of reply. My original letter was mailed back to me from what must have been the editors' assistant, a Mrs. Marge Williams, with the addition typed upon the letter and highlighted with the date 1/25/77: "Sorry you did not receive an acknowledgment card. We did receive your manuscript and apologize for the inordinate delay in responding with reviews of your manuscript. We have run into trouble with procrastinating referees and have at this time are awaiting one more review."

Some time in April 1977 Melvin Tobias, Associate Editor of Nuclear Science and Engineering, called to tell me that he was having a difficult time finding more individuals who would agree to review the manuscript on April 14, 1977, I sent him a list of ten potential reviewers with detailed mailing addresses. I summarized after this list "The basic problem that reviewers have with the analysis in the paper is that a proof of our claims in the form of a mathematical theorem is not given and may not even be possible in general. The paper has been proven useful to investigators who appreciate that there may be difficulties solving partial differential equations having complex characteristics as an initial value problem. We demonstrate that under certain conditions, a stable (well-posed) solution may not be possible to generate." This in a nutshell was the message of the paper which we did not explicitly state.

I included (1) a copy of the Boure et al. and Ishii written discussions and my rebuttal (Appendix E) circulated at the session at which I presented our paper at the ASME Winter Annual Meeting in 1975; (2) the late arriving discussion of Moody et al. summarized above; (3) two pages from the recent paper by Travis et al. with the statement on page 5 which I highlighted: "In the absence of viscous dissipation, the equations exhibit an instability growth rate that becomes infinite as the perturbation wavelength becomes vanishingly small" [11] which refer to the ill-posedness of the two-phase equations; and (4) a copy of Dimitri's Introductory remarks prepared for the NSF Workshop Mathematical Modeling held at the Two-Phase Flow and Heat Transfer Symposium-Workshop held in Fort Lauderdale, Florida, October 18–20, 1976. The findings of this Workshop were eventually published in 1978 [12]. I also included a copy of Dimitri's Roundtable discussion presented at the Fifth International Heat Transfer Conference [2]. I drew attention to a portion of Harlow's reply on page 166 referring the Lax's "high-frequency test" to determine whether a formulation of two-phase equations is properly posed.

In a letter dated April 20, 1977, Melvin L. Tobias the Nuclear Science and Engineering sent me the first review of our manuscript. It consisted of two pages, single spaced, and separated into ten separate comments. They were obviously written by someone intimately familiar with the history of the characteristics issue for one-dimensional two-phase flow. In comment (5), the reviewer took issue with using characteristics analysis. He stated "…it is [sic-the word *not* is obviously missing] advisable to look at characteristics at all—one should instead use the 'high frequency test', i.e., assume a solution of the form exp i(kx-wt) in the linearized equations and see whether unstable growth occurs as k → ∞." He continues "The characteristics controversy has been carried on in the reactor-safety community for over 2 years now, and it is now generally accepted that the high frequency test is the appropriate way to analyze the equations." In comment (6), the reviewer took issue with the second paragraph of the manuscript in which "…the authors seem to be hinting that real characteristics are an argument in favor of an equation set. In fact this view seems implicitly to pervade the entire manuscript." This paragraph referred to contains a litany of references to authors who either have the volume fraction inside or outside of the pressure gradient. He takes particular pains to point out that one of the authors referred to in our paper, Harlow and Amsden [13] "…mention the important point…that equations with α^a [volume fraction of phase a] inside the pressure gradient fail to perpetuate hydrostatic equilibrium and must therefore be rejected regardless of their characteristics behavior." In effect, he is not only criticizing us, he is damning the other authors who use this form of the pressure gradient. We did state in the manuscript that the Harlow and Amsden [13] consider this form as unrealistic. In comment (7), the reviewer criticizes the addition of transient flow forces to the basic equations since as pointed out in the report by Ramshaw and Trapp [14] (we referred to it as being submitted for publication in Physics of Fluids in 1975 which was corrected by this reviewer) "…the uncritical introduction of such terms can suppress physical instabilities." This comment ends by again insisting that the high-frequency test be utilized rather than characteristics. In comment (8), the reviews again cites Ramshaw and Trapp to justify adding higher-order terms like surface tension and viscosity render the equations well-posed yet allow for physical instabilities. Comment (9) questions the entire thesis of the paper. We were only acting as reporters of our analysis and not any high flying issues such as "careful examination of the physics." In comment (10), the review concludes that "From the above comments, it is clear that the paper cannot be published in its present form." He ends his damning with faint praise by stating "…the authors have clearly done a lot of work and it appears that much of their experience might be of value to others, provided that it is reinterpreted in the light of generally accepted current knowledge as discussed above." From the frequent references to Harlow's papers, this reviewer must have been a member of Group T-3 at LANL. This suspicion is reinforced by repeated insistences advocating the use of the high-frequency test rather than characteristics. The Group Leader of Group T-3 at the time this review was written had become Tony Hirt, who replaced Frank Harlow in 1974. Because of the references to Ramshaw and Trapp's report (published in 1978) [14], I include in Appendix F an unpublished commentary sent to me by John Ramshaw as a personal communication which summarizes his final thoughts on this paper. Ramshaw and Trapp's initial viewpoints were published in 1974 for Dimitri's Roundtable Discussion at the Fifth International Hear Transfer Conference [2].

By the time I received the second set of two reviews in August, 1977, I had already left Energy Inc. on June 17, 1977, to join Lawrence Livermore Laboratory, now Lawrence Livermore National Laboratory. These two rather short reviews were rather bizarre in that they referred to the first reviewer's comments discussed above! Both reviewers concurred that the paper could be published with extensive revision as suggested by first reviewer. In essence, they simply summarized what our manuscript contained and made a number of suggestions for the revised manuscript. One reviewer stated that the conclusions arrived at in the manuscript are useful as are the appendices. On September 2, I sent a letter to Melvin Tobias thanking him for his fair and unbiased review process and for his patient considerations. I assured him that the revision could be revised to incorporate responses to the reviewers' comments without a major rewrite and without a significant increase in length. In addition the revision would include reference to research performed since the original presentation of our findings. I responded to the reviews with a revision of the manuscript on November 30, 1977, by doing a cut and paste of the ASME reprint by adding text which addressed the reviewers' comments and by adding a new section called RECENT DEVELOPMENTS. I explained in detail the revisions which were made to address the ten comments made by the first reviewer. In January 1978, I received a form from the ANS informing me that “The editor has released your manuscript for publication in Nuclear Science and Engineering. After copy editing and typesetting, page proofs will be sent to you for checking and final author approval of the processed paper.” The paper was finally published in 1978 [15]. I received a smattering of requests for the paper from the USA and abroad. As I already mentioned above, it has garnered 207 citations and counting in Google Scholar. So, the publication history of the characteristics paper straddled no less than three employers and 5 years. And as they say, the rest is history…at least with respect to the complex characteristics issue. The second paper proposed in my letter to Dixon Callahan in my submittal of the characteristics manuscript on September 8, 1976, evolved into two papers published in 1978 and in 1979 [16, 17].

I have to include something enlightening about Zuber’s attitude toward complex characteristics. EPRI held a Workshop on Basic Two-Phase Modeling in Reactor Safety and Performance, Tampa, Florida, February 27–March 2, 1979. The list of participants is a Who’s Who of experts in all phases of two-phase flow research, including Brian Spalding. I was not invited, but Dan Hughes, still at Energy Incorporated, and Charlie and Vic from EG&G Idaho, were. In 1980 EPRI published a two volume Proceedings (EPRI WS-78-143) [18] containing transcripts of the discussions and presentations, some of which appeared in a special issue the International Journal of Multiphase Flow in 1980 [19]. Zuber got the last word in on the issue of the complex characteristics: “…this problem of hyperbolicity and ill posedness. It exists, I don’t think it’s a big problem. We can go around it by proper averaging…There is no problem. So that problem—if it arises—really to cause a problem in the future for the code can be removed rather easily.” Three Mile Island accident occurred on March 28, 1979, which resulted in the end of nuclear power construction to this day. It was not the result of a LOCA but of what is termed a small break accident.

During the writing of this chapter, I happened to find, by performing a Google search of the internet, the book by Herbert Stadke relating to hyperbolicity [20]. There are no references to our paper [15] and subsequent publications, nor to any publications by Dimitri including the seminal Roundtable Discussion [2] and his first book [21], nor to any fluidization literature for that matter, and absolutely nothing from Los Alamos. The references cited are highly selective and quite dated except for some of Stadke’s more recent publications. In Chap. 3 he immediately restricts the scope of his book to single-pressure models stating on page 38 “Although all of these ‘two-pressure’ models show interesting aspects of two-phase flow, they are valid only for specific flow regimes or for a limited range of flow conditions. None of them has yet reached a state of maturity for broader applications to scientific or technical problems. This is the reason why in most of the present two-phase models of two-phase flow, the assumption of equal local pressure for the two phases is introduced [gas pressure = liquid pressure = interfacial pressure]. This seems to be justified for many technical applications as long as surface tension effects are neglected.” Included in the two-pressure models Stadke refers to is the model of Ramshaw and Trapp [14] and Ransom and Hicks. [22]

Ramshaw, Trapp, and Ransom were participants in the SLOOP code development, and Ransom went on to develop RELAP5 (not referenced) which employs added mass to partly reduce the areas of complex characteristics that result from having the void fraction outside the pressure gradient in the momentum equations [15].

In Chap. 4 “Simplified Two-Phase Flow Models,” Sects. 4.1 “Homogeneous equilibrium model” and 4.2 “Homogeneous nonequilibrium two-phase flow,” Stadke obtains the characteristics which were obtained in Appendices C “Homogeneous Equilibrium Model” and B “Derivation of Homogeneous Mixture Sound Speed Using Method of Characteristics,” respectively, of our paper [15] to which he does not refer. He proceeds then to obtain the characteristics for what he refers to as the “Wallace model” in his Sect. 4.3. These are the same momentum equations analyzed in our paper [15] and given in Chap. 6 above by Eqs. (6.1) and (6.2). He verifies our results that this equation set (1) possesses complex characteristics for the case of both phases incompressible and that (2) for equal phase velocities the characteristics are real. These results agree with the results given in our paper [15] and given by Eqs. (6.8) and (6.11) in Chap. 6. Stadke concludes on page 71 “…that the ‘Wallace model’ has not a complete set of real eigenvalues” with his opinions on the dire consequences: (1) “the model does not represent a ‘well posed’ initial-boundary value problem,” (2) “…all numerical techniques developed for fully parabolic systems of equations cannot be applied,” (3) “the model does not realistically describe pressure wave phenomena…and critical flow predictions,” and (4) “…short wave length instabilities require specific damping mechanisms in order to obtain stable numerical results.” The final statements on this page are particularly damning and include: “Despite these disadvantages, the Wallace model is still the basis for many of today’s two-phase flow computer codes. …However this is compromised by the severe inaccuracy in predicting local flow quantities, especially in the presence of large density or void fraction gradients.” These claims give the reader the impression that they have been substantiated by the author albeit no results or references are given. In Chap. 5 “A Hyperbolic Model for Two-Phase Flow,” which contains new results, Stadke uses a modification of the transient flow force given by Eq. (27) in our paper [15], to force the characteristics to be real. Stadke states on page 77 that “Rather comprehensive algebraic studies have been performed to verify the effect of the open parameters… on the eigenvalues…This required an enormous amount of algebraic manipulations…” This result is an interesting result, and the implications will have to withstand the test of duplication and criticism by the two-phase flow community.

Stadke is like a host of authors studying the two-phase flow complex characteristics issue. They totally refrain from referring to our groundbreaking work on the subject in hopes of giving the impression that they themselves have discovered the problem. Instead of dismissing outright equation sets in deference to his hyperbolic model, he should compare the models to analytical solutions and experimental data to discriminate among them.

The moral of this chapter is, if you have the courage of your convictions, even if the odds appear insurmountable, be persistent and honest. New and controversial results will always encounter hostile critics defending their "conventional wisdom." If the length and detail of the characteristics paper history in this chapter annoys the reader, I apologize. At least it is not as long as the author of "Faster than the Speed of Light" [23] which required a 277 page book to trace the history of his attempt to get his manuscript on the varying speed of light (VSL) theory published!

It would be remiss if I did not learn something by spending such a great deal of space discussing the complex characteristics problem in this book and with Dimitri. Based on this process, we are convinced that two-phase models should have all the pressure drop in only one phase, either gas or liquid, because these models are well-posed. We knew this in Idaho during the SLOOP code development when I worked on developing the extended Rudinger-Chang model [24–26] discussed in Sect. 7.3. This model was not adopted because of the objection due to the necessity of switching phases.

Two-phase flow models that have the same pressure in each phase are incorrect for dispersed flow. The reason for this is that since there are discontinuities across the phase interface, *derivatives of pressure for the dispersed phase do not exist*. The kinetic theory of granular flow [21] resolves the problem of ill-posedness because it presents a clear explanation of the concept of pressure. It makes no sense to have a gas-phase pressure drop in the solids phase because the collisional pressure drop is small. This is a critical issue since all commercial codes have the pressure drop in both phases which can lead to instabilities when the viscosity is small.

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Part III
The Rise of CFD Codes

Wherein is told of developments at the NRC, DOE, EPRI, and IIT of the rise of multiphase codes for nuclear reactor safety and energy analyses.

Part III describes what preceded the widespread application of the two-phase seriated continuum approach (later referred to as the two-fluid or interpenetrating continuum model) outside of the US National Laboratories and international research institutions, such as existed in the UK, France, and Canada (mainly nuclear and defense related). Only they possessed the large expensive mainframe computers required to solve these equations numerically. Private companies, such as Control Data and Boeing, were leasing available computer time on their mainframes, but it was expensive. Energy Incorporated where I spent two years after leaving ANC started its business by leasing computer time and eventually bought its own mainframe. Larger universities, including IIT, would buy their own mainframe computers to support their departments' research. Later the National Science Foundation (NSF) would establish supercomputer centers at several universities. In time, advancements in the integrated circuit would make it possible to solve such equations on increasingly inexpensive and powerful personal computers (PC), high-end workstations, and clusters of PC's. The capabilities of what were called mainframes in the 1970s and 1980s would be exceeded by orders of magnitude. Coinciding with the rise of the integrated circuit technology was the rise of the Internet and the World-Wide Web which made it possible for much faster communication among researchers and much more rapid dissemination of information and publications.

Chapter 9
RETRAN Is Initiated at Energy Incorporated for EPRI Hiring the Core SLOOP Code Participants

Chuck Rice was replaced as General Manager of ANC on May 15, 1972, and shortly thereafter founded Energy Incorporated (EI) on June 12, 1972, as its President. I left the SLOOP code project at ANC on July 14, 1975 (Bastille Day), and started at EI in the morning of the very next day. I was preceded by just a couple of weeks, or less, by Dan Hughes and Jim McFadden. Ken Moore the key developer of the RELAP series of nuclear reactor safety codes was lured away from ANC in 1974 to join EI. He provided RELAP4 consulting expertise for ANC, thereby filling the void created when he left as Supervisor of the System Model Optimization Section in Charlie's and later Vic's Analytical Model Development Branch. When I joined EI, there was already a whole host of key ANC personnel who had been lured away. There was George Niederauer and John McClure, who both worked under Ken Moore in the Containment Modeling Section, and Kent Richert who sometimes assisted on the SLOOP code checking out friction correlations. Even Don Curet who was Manager of ANC's Systems Analysis Applications Branch was already in charge of Program Coordination under Roger Griebe, head of EI's Systems and Analysis Branch which included all of the technical activities including Ken Moore's section. Maybe lured is the wrong word. The hostile and negative criticism generated by the AEC RSR in their review meetings as discussed in Chap. 7 was probably the overriding reason why all of these fine people left. This haranguing by the RSR had continued into 1975. We all left for pretty much the same reason, disgusted with the AEC then the NRC RSR tactics. I was initially assigned to Ken Moore's Thermal Hydraulics Section upon joining EI along with Dan Hughes and George Niederauer. Jim McFadden went into Kent Richert's codes section. I had no regrets leaving the disjointed, confusing atmosphere at ANC. It was a roller coaster ride I hoped would never happen again. I stayed at Energy Incorporated for what would be an interesting, creative, and productive almost exactly 2 years. I was assigned to quite a wide variety of projects. I will summarize just a few of my major contributions to them in this chapter.

R.W. Lyczkowski, *The History of Multiphase Science and Computational Fluid Dynamics*, Mechanical Engineering Series,
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Energy Incorporated was a consulting company located in a three-story bank building in downtown Idaho Falls and catered almost exclusively to the nuclear industry. When I joined EI, the Electric Power Research Institute (EPRI) was its largest single customer. EI supplied consulting services to ANC, Argonne National Laboratory West, US electric utility companies who operated nuclear reactors, and manufacturers and construction companies who built them including Bechtel Power, Babcock and Wilcox, General Electric, and Combustion Engineering. These services were also supplied to operators of nuclear reactors outside the USA including Canada, Japan, Denmark, and Germany.

My very first assignment less than a month after joining EI and settling into my office was to work on a contract with the Institute fur Reaktorsicherheit (IRS) located in Cologne, Germany. It involved programming the IRS subcooled critical flow or choking model into RELAP4 which was installed on their computer. I was to travel there with John McClure who was in EI's Physics Section. I was probably chosen because I know about critical flow having simulated such test problems at ANC, as well as having simulated Standard Problem 1 with both the EVET and UVUT codes. In preparation for the meeting, I studied all about the subject of subcooled critical flow and had to get familiarized myself with how to run RELAP4 installed on EI's computer. John McClure was to do the programming, and I would try to understand the proprietary IRS choking model. The problem was that all of the documentation was in German authored by the person who developed the model, a Dr. Peter Pana (yes that really was his name). The work was originally scheduled to be finished by August 16. However, I was going to present two papers at the 15th National Heat Transfer Conference held in San Francisco, August 10–13, 1975: "Pipe Blowdown Analyses Using Explicit Numerical Schemes, [1] and Transient Propagation Behavior of Two-phase Flow Equations" [2] and also to chair the session Heat Transfer in Reactor Safety. EI graciously allowed me to attend this meeting and so alerted IRS that the work would not be able to begin the work in Cologne until August 25 after the Heat Transfer Conference. The schedule for the contract was very tight allowing for only 2 weeks effort at EI and 2 weeks in Cologne.

I can't remember how it came about, but I managed to get myself an invitation to visit Jean Marc Delhaye and his group at the Service des Transferts Thermiques (CENG) in France. I told them I could do that after I finished my work in Cologne. They agreed and EI agreed. So, after my work was done in Cologne (much drinking of Kolsch beer at the local bars and at the IRS headquarters where one day somebody tipped over his beer into the computer printer), I travelled by train from Cologne to Grenoble over the French Alps which was a very scenic ride. I had a great time in Grenoble spending September 8–9, 1975, there meeting with Jean Marc Delhaye, Jean Boure, and a host of others in Delhaye's group. Boure was very excited that EI had access to all of the codes developed at ANC and said he would like EI to present a proposal to CENG using the SSUVET and/or the SSUVUT codes to check out his critical flow theory. I told him that I would work on the proposal when I got back to EI and then we could go over it when Delhaye and Boure visited Idaho Falls on October 7, 1975, after what was billed as the

Third NRC Water Reactor Safety Meeting, to be held in September 29–October 2. The first two such meetings which must be considered to be the first two were the March 17–19 and June 11–12, 1975, NRC meetings discussed in Chap. 7. I returned to Cologne by air from which I returned to Idaho Falls. After I got back to EI, I drafted a report documenting the subcooled choking flow work for IRS in an EI Corporation Confidential report and the minutes of my trip to CENG.

Next I wrote the proposal titled Unequal Phase Velocity, Unequal Phase Temperature Two-Phase Critical Flow Studies for CENG and it was sent to Delhaye on October 1, 1975, in time for our meeting in Idaho Falls on October 7. This was in addition to all the preparations for the presentation of the paper "Characteristics and Stability Analyses of Transient One-dimensional Two-phase Flow Equations and their Finite Difference Approximations", which was to be presented at the Winter Annual ASME Meeting, in Houston where Delhaye, Boure, and I would meet once again [3]. For a discussion of this meeting, the reader is referred to Chap. 8. I proposed a 22 man-month effort to be completed in one calendar year. It turns out that CENG never really intended to fund any work at EI and so it was just a big ruse. CENG sent a letter to EI on January 23, 1976, stating that "…it is not possible to give you a contract for work which seems to us a little premature." I suspect that the experience in Houston discussed in Chap. 8 and the influence of Tong, Fabic, and Zuber at the NRC had a great deal to do with CENG's reneging on cooperation with EI and the warding of a contract.

The three of us Dan, Jim, and myself, plus George Niederauer, started to work on a contract to EI to write a report for Lance Agee, project manager at EPRI, documenting the work that was done at ANC during the three-and-half year SLOOP code project. Why was he so interested in such a project? Lance Agee almost joined Charlie's SLOOP code project in 1974. Lance sent his resume to ANC sometime in 1974. At the time he worked for Combustion Engineering in Connecticut. He came out for an interview and was given high marks by everyone involved and so received a job offer. Lance was quite excited about our efforts. Lance accepted the offer and put his house on the market. It was late in the year, around November, or December 1974. Selling a house during the holiday season and into the winter proved to be a difficult matter. Someone in management decided that it was taking far too long for Lance to report for work and demanded that he show up by the end of December 1974 or the offer would be revoked. He was not successful in selling the house, he didn't report for the job, and the offer was rescinded. He was eventually hired as a project manager at EPRI in 1975. Dimitri tells me that Charlie was made an offer by EPRI at about the same time frame to be a project manager. He declined the offer. Had he joined EPRI, the story in this book would have been considerably different. He might have gotten Agee's job. Agee would become the project manager for most if not all of the subsequent code development work over the years at EI. We started writing the report which must have taken most of 1975 going into 1976. It was typed on EPRI camera-ready mats and published in February 1976 as three separates volumes [4–6]. Dan Hughes tells me it was one of EPRI's best selling reports. These three volumes were collected together and reprinted as a single volume with the same publication data.

The next project I worked on for most of my remaining tenure at EI related to the development of the RETRAN computer code under the direction and sponsorship of EPRI with EI as the major contractor. Agree was the project manager and guiding hand in its development. The first documentation of the code was published in 1977 [7]. RETRAN is a state-of-the-art computer code developed primarily for licensing and safety analyses for the electric utilities' nuclear power plants. It is designed to analyze a wide variety of fluid flow and heat transfer problems for complete nuclear and fossil power plant systems. The code solves the one-dimensional HEMM model describing steady and transient one-component two-phase compressible flow systems coupled with heat-conducting structures. As far as I could tell it is an improved version of RELAP4 and initially had the same solution technique. It is also designed to analyze nuclear plant operational transients, small-break LOCAs, and balance of plant transients. RETRAN achieved wide acceptance by the nuclear industry. It has been licensed to all US utilities that have nuclear power plants, consulting firms, universities, and government agencies which sublicensed the code to national laboratories to assist them in running it for them.

When I was at ANC, I started to work on mechanistic models which could be used to derive the drift velocity in the so-called drift model of two-phase flow utilizing some of the correlations for the SLOOP code frictions models. These steady-state slip models were then programmed into the HEMM momentum equations in the RELAP4 code [8]. They could also be used in the UVUT-DF version of the LOOP code [9]. Then I analyzed the characteristics of RELAP4 with slip to find the conditions under which the eigenvalues would be complex and presented the results at the ANS 1975 Winter Meeting in San Francisco, November 16–21 [10] just a week before presenting the paper "Characteristics and Stability Analyses of Transient One-dimensional Two-phase Flow Equations and their Finite Difference Approximations" in Houston [3]. EI allowed me to attend both meetings. It occurred to me that this idea could be extended by manipulating the difference between the two-phase unequal velocity momentum equations used in the SLOOP code to derive a transient equation which could be used to solve for the slip velocity. I coined this equation the "dynamic slip model" which was sort of sexy. I was able to convince Ken Moore, who was a very conservative but bright person, that such a model could be used to improve EI's version of RELAP4. It was straightforward to insert the necessary modifications for the so-called implicit FLASH numerical method of Porsching et al. [11] used in RELAP4 to solve for the mass, momentum, and energy equations. The dynamic slip equation was backward differenced in time to solve for the slip velocity and added to the code which came to be called RELAP/SLIP in preparation for analyzing NRC Standard Problem 6 [12].

Next several test problems were run that would be impossible to simulate with the HEMM equal phase velocity model in RELAP4 [12]. This included the classic situation of an enclosed vessel with a volume of water initially situated over volumes of steam. The HEMM model would only compute a slight compression of the steam with the water remaining on top. This is referred to as the "water stacking problem." With RELAP/SLIP, the water descended to the bottom with a slight oscillation of the enthalpy when the volume completely filled. For the inverse problem of a volume of steam representing a bubble rising through two volumes of water above it, the steam rose to the top and when the water filled the bottom volume there was an oscillation of the water volume fraction. These oscillations are related to the problem of "water packing" which occurs when a volume of water exits a control volume. RELAP/SLIP was exercised by running several more problems including NRC Standard Problem 5 based on Semiscale blowdown heat transfer test S-02-8 [12]. Ken Moore was ecstatic over the test problem results with RELAP/SLIP, and so it was to be used to simulate a priori NRC Standard Problem 6 based on Semiscale blowdown heat transfer test S-02-6 [13]. As far as I can determine, this report was never issued for some reason. Del Mecham and I worked closely together on the development and checkout of the dynamic slip model [12]. He was the lead on the project and was responsible for modifying the RELAP4 HEMM equation to include slip, programming the dynamic slip model, and running the simulation of Standard Problem 6. He used this material for his doctoral thesis for which I was his de facto advisor [14]. However, I was not on his thesis committee which approved his thesis. Figures 116, 117, and 136 through 139 in Del's thesis for the core inlet density and rod temperature demonstrated the power of the dynamic slip model [14]. Without dynamic slip, the core uncovers, the lower plenum flashes, and the result is a rapid and high heat up of the heater rods. With dynamic slip, countercurrent flow in the core and downcomer regions allows vapor to escape while liquid remains and covers the core. Therefore, the heater rods remained immersed in water and surface temperatures decrease monotonically essentially maintaining saturated liquid temperature. The dynamic slip model and key simulations including the one just summarized were eventually published in a peer-reviewed paper, and as an homage to Charlie, I included him as an author [15].

My two contributions to the development of RETRAN were documented in Volume I of the code manuals published in 1977 [7]. The first is the dynamic slip model which was refined and then programmed into the RETRAN code to transform it into a pseudo-UVET code as documented in Section II 4.0. The experience shaking it down in RELAP4 described above proved invaluable. The second is the extension of the so-called implicit FLASH numerical method [11] used in RELAP4 as documented in Section VIII. In reality, the FLASH technique is an *explicit* numerical scheme even though Porsching et al. refer to it an *implicit* scheme because the variables in the Jacobian matrix in the quasi-linearization of the HEMM equations are held back at the old time level. I hit upon the idea of extending the explicit quasi-linearization scheme into an iterative scheme, which, when converged would solve the nonlinear HEMM equations. This concept was first tested in RELAP4 and presented at the ANS 1976 International Conference in Washington, DC, November 15–19, 1976 [16]. This coupled with rational time step control and improvements in the explicit numerical scheme sped up the running time for the RETRAN code by at least 25% and usually considerably more [17]. Techniques to address the resolution to the water packing problem were developed, but I'm not sure they were implemented in RETRAN [18]. These two papers, as well several more by Charlie and colleagues at EI, were presented at the local chapter of

American Nuclear Society Thermal Reactor Safety Meeting in Sun Valley, Idaho, July 31–August 5, 1977. They appeared in the Proceedings [17, 18], but were never published in a peer-reviewed journal.

I'll just briefly mention three other activities I was involved with that related to multiphase flow while I was at EI. The first activity was an interaction with Systems, Science and Software, (S^3) a consulting company that was in La Jolla California. They received a contract from ERDA in 1975 to develop a multidimensional computer program for fluidized bed gasifiers using what they termed the interacting continua approach. This is basically the same concept as the seriated, or two-fluid, model of two-phase flow. EI became aware of this effort in late 1975 and contacted one of the investigators, a Dr. M. F. Scharff. I was drawn into the situation and contacted Dr. Thomas Blake by phone in April 1976. He told me Scharff had been the project manager for the ERDA contract titled Computer Modeling of Coal Gasification Reactors but had left for JAYCOR another consulting company located in Del Mar near San Diego and had taken over his position. He was cognizant of EI since a couple of EI representatives visited them in January. There was some interest in collaboration. Tom Blake called me in May 1976 and expressed an interest in visiting EI in July after an ERDA program review in June. He wanted to pursue possible joint proposals. I don't recall his ever having visited EI. I believe they fell into serious programmatic difficulties and then lost interest. More details will be discussed about the S^3 and JAYCOR computer modeling projects in Chap. 11.

Around this time I decided to write the paper documenting the UVUT simulation of Standard Problem 1 discussed in Chap. 7. It was my intention to present it at the 1976 Heat Transfer and Fluid Mechanics Institute Meeting in Davis, California, June 21–23, 1976. In my submission of the manuscript to the general meeting chairman in November 1975, there were seven authors listed in the same order as in Vic Ransom's transmittal of the report [19]. It was then circulated for comments by the coauthors. There was quite a heated discussion at a meeting at EI, with the President Chuck Rice presiding, concerning the ordering of authors. It turns out everybody except Charlie and I disagreed on the author ordering. Chuck Noble and Bob Narum became particularly nasty. They thought that without them the SLOOP code would have never been programmed. Chuck Rice sliced through the rancor and then we tried to divine who were to be the principal authors. It came down to the following order: Charlie, Glen Mortensen and me. Charlie because he started the SLOOP code effort, Glen because he listened to me and programmed the flashing model I developed as discussed in Chap. 7. Charlie and I responded to the reviewers' comments and I submitted a revised manuscript to the General Chairman at the end of February. EI allowed me to attend the meeting at which I presented the paper. It was published in the Proceedings made available shortly after the meeting [20].

The second activity was due to Dimitri's involvement with organizing what turned out to be the first Two-Phase Flow and Heat Transfer Symposium-Workshop held in October 18–20, 1976, in Fort Lauderdale, Florida. It was sponsored by the

National Science Foundation and the School of Continuing Studies at the University of Miami. There were to be four more such conferences over the next 12 years finally becoming the Miami International Symposium on Multi-Phase Transport & Particulate Phenomena. The conference series ended with the fifth in 1988. I received a personal invitation from T. Nejat Veziroglu Director of the Clean Energy Research Institute at the University of Miami in February 1976. He chaired the Organizing Committee on which Dimitri was a member. I sent a two-page abstract to Veziroglu in March with a copy to Lance Agee. I really went all out for this meeting. I proposed nothing less than a critical review of numerical techniques for the computation of transient unequal phase velocity unequal phase temperature (UVUT) two-phase flows. Dimitri, who was assisting in reviewing the abstracts for the meeting, suggested that I revise the abstract which I did. It expanded to slightly over three pages. In June, the paper was accepted for presentation. He instructed me to prepare an extended abstract which would be published before the meeting. In July, I sent the extended abstract to him, which was just a reformatted version of the revised abstract prepared for Dimitri, along with my short biography. I presented my paper on October 19 which was the last one in the session Two-Phase Heat Transfer. The meeting was attended by some of whom I refer to as "all-stars" in the area of two-phase flow: Art Bergles, who gave the Keynote Address "Two-Phase Flow and Heat Transfer, 1756–1966", S. L. Soo, Mamoru Ishii, Joel Weismann, Hans Fauske, and George Yadigaroglu. Charlie presented two papers with Dan Hughes, Dan Hughes presented one, and Rex Shumway presented one, and so ANC (replaced by EG&G Idaho in 1976 by the time of the meeting) was well represented. Dimitri held a "Mathematical Modeling Workshop" on October 20, the last day of the conference, which addressed unresolved mathematical modeling problems in two areas: (1) advanced computer codes for licensing nuclear reactors—problems with separate phase momentum balances and drift flux and (2) scale-up of coal conversion processes. I attended Dimitri's workshop which had Clayton Crowe, S. L. Soo, and Thomas Hanratty offering constructive discussions. As I remember, Brian Spaulding also played a prominent role in this workshop.

I worked on the paper off and on after the meeting and submitted the manuscript to Veziroglu and a copy to Lance Agee in February 1977. It contained a review of all the two-fluid computer codes I was aware of (some two dozen plus) from 1964 to 1976. I also summarized the various solution techniques including as best I understood those from developed at LASL. It was quite an effort. The paper was published in Volume II the Proceedings in 1978 [21].

The third and by far the most interesting activity was working as a consultant to EG&G helping them to analyze flow in the cold leg blowdown pipe of the LOFT experimental facility during a LOCA. The basic problem was that the measurement techniques to determine the transient mass flow in this pipe; drag disk, turbine flow meter, and gamma-ray densitometer; were inconsistent and disagreed with the water collected in the suppression tank. Therefore, there needed to be a better understanding of what the flow structure was in this pipe. It was proposed to use the K-FIX computer code to compute the two-dimensional velocities of the water and steam and their volume fraction during the blowdown. This information would serve to provide a more reliable reduction of the data. The K-FIX code had been under development at LASL and was about to be documented [22]. INEL had received the code and had it installed at the INEL Computer Science Center (CSC). It was proposed that several improvements to K-FIX were to be made to achieve a more realistic simulation. I was chosen to consult on this project because I had worked on the SLOOP code, was familiar with the developers of the K-FIX code, and was instrumental in improvements to RELAP4 and RETRAN including a more realistic flashing model to analyze NRC's Standard Problem 6. I clearly recall that Jim Lime, office mate of Wen Ho Lee at the CSC, was unsuccessful in reproducing Standard Problem 1 reported by LASL using the K-FIX code [23]. The subcontract to EI was negotiated in March 1977. I then proceeded to work closely with Paul Demmie, who performed the simulation with my advisory supervision. This allowed me to become more familiar with the code which would play a role in initiating Dimitri's IIT code as discussed in Chap. 13. Paul's report was published long after I left EI [24]. However, I did receive a nice acknowledgment.

Before leaving EI, I would meet with Wen Ho Lee at a nearby restaurant to collaborate on a paper we had started writing when we were both at ANC. He was hired in 1974 by Larry Wheat to work on what was called the BEACON (Best-Estimate Advanced COntainment) computer code. Wen and I started up a friendship which has lasted to this day. He once invited me to go fishing with him, an activity in which I never actively pursued. He taught me how to fish. He said to drop the line near rocks where the fish were supposed to congregate. If they didn't bite, move on to the next collection of rocks. He caught about a dozen fish and I caught about a dozen. After we got back, Wen fried them and we dispatched them heartily. We both like classical music and gardening. We are kindred spirits, reluctant to obey authority and willing to follow the courage of our convections to innovate and strike out on our own. I contributed some ideas on test problems for the code. I suggested the gravity settling problem. Lee wrote a paper and submitted it to the 17th National Heat Transfer Conference which was to be held in Salt Lake City, August 14–17, 1977. It was published in the AIChE Preprint volume [25]. We would expand upon this paper in later years and eventually I managed to get it published [26]. I also wrote a paper for this conference with Charlie which would also eventually be published [27] based on some work I did at ANC to check out the UVET code.

Although I was able to attend quite a few meetings (two in 1975, and four in 1976) and was encouraged to publish (EI would give an honorarium for each paper published in proceedings and peer-reviewed journals), I was not entirely comfortable working for a consulting company. Everyone was out to protect their job. They were reluctant to tell you what they were working on or leads they had to snare contracts. I didn't have any contracts of my own and was working for those who did. I interviewed Lawrence Livermore Laboratory (LLL) in 1976 in response to an ad for work in the underground coal gasification (UCG) project, encouraged by Dimitri. After a substantial delay, I received an offer in 1977 and since it was such a long time since my interview, I said I needed to visit LLL again. That I did and was subsequently impressed that it would be a good opportunity to work on some multiphase problems associated with UCG. I sold my Corvette and Cadillac and put up my house for sale which sold promptly. I then resigned EI on June 19, 1977, had my household goods loaded into the moving van, and then drove to Livermore in my Audi. It turns out I found out that Joe Ching with whom I worked at EI was also leaving. He was going to teach in the Nuclear Engineering Department at the University of California Berkeley. We would become “partners in crime”, so to speak, once we were settled in. I started employment on June 20, 1977. As I was driving over the hills separating the Livermore Valley from the Pacific coast, I was caught for speeding since I was anxious to get to the “land of milk and honey.” I got off with a warning and drove on. In a short time, I was able to purchase a house in Livermore close enough to ride my bicycle. And so the saga of Idaho Falls was history. I have never returned.

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Chapter 10
RELAP5 is Initiated by Vic Ransom and Dick Wagner Funded by Larry Ybarrondo

After I left the SLOOP code at ANC and joined EI, my contacts with John Trapp, Bob Narum, and Chuck Noble, who remained behind, stopped completely. My interactions with Vic Ransom dwindled because I was extremely busy at EI and, when we did meet, they were purely social. I didn't want to talk about what happened to the SLOOP code after it imploded, and I don't think Vic did either. I would get together with him and his wife at his farmhouse located on quite a few acres outside of Idaho Falls. I would bring over my classical records and listen to them on his fancy stereo system. He had bought an amplifier with a built-in four-channel quadraphonic decoder. Once I lugged over two of my speakers, hooked them up to his amplifier and we listened to four-channel reproduction from the quadraphonic records I had purchased. He told me much later that it was I who introduced him to the woman who would become his second wife. He had divorced his first wife in California before he joined ANC in Idaho Falls. As mentioned in Sect. 6.2, I bought a small two-story house in Idaho Falls which I rented out and also managed myself. The house had completely separate entrances for the basement apartment, which was furnished with a kitchenette, and for the ground floor apartment. One time after I rented the latter apartment to two women, they started to paint some of the rooms in garish color combinations which I strongly objected to. One of the women, Delrie Gridley, was very outspoken. She told me in no uncertain terms that they could paint the rooms, however, they wanted and told me where to go. I mentioned this story to Vic during one of the parties at my home and he asked me for Delrie's telephone number. He dated her, and they married soon thereafter. I went to their wedding in Pocatello shortly before leaving ANC to join EI.

When I was at EI, I was totally unaware that Vic was developing RELAP5 since he never mentioned it to me, and I had no business with ANC's Analytical Model Development Branch. My contact with Vic ceased completely when I left EI in Idaho Falls and joined LLL in Livermore, California. Consequently, I was never even aware that RELAP5 existed until decades later. It was sometime in the 1990s that Vic was invited by the Reactor Analysis and Safety (RAS) Division at Argonne National Laboratory to give a seminar while I was in the Energy Systems Division.

R.W. Lyczkowski, *The History of Multiphase Science and Computational Fluid Dynamics*, Mechanical Engineering Series,
https://doi.org/10.1007/978-3-319-66502-3_10

The seminar probably had to do with Vic's experience with developing RELAP5. Before the seminar, I went up to him to shake his hand, establishing the first contact with him since I left Idaho Falls. It was then that I learned that in 1990 he had joined Purdue University in West Lafayette, Indiana as a full Professor and Head of the Nuclear Engineering School. I was impressed. After the seminar, I chatted with Vic. I told him what I was working on computer modeling of fluidized beds for a project for a consortium interested in addressing the erosion problem in fluidized-bed combustors. I didn't have much time to ask Vic about details of his work on RELAP5 as he was being rushed off to talk with personnel in the RAS Division who were working on code development for fast breeder nuclear reactors. After he left, I asked somebody in the RAS Division if they could get me a copy of the RELAP5 code manual [1]. After I received it, I filed it and then forgot all about it until writing this book. By the time I met Vic at ANL, he had grown a beard probably to appear more professorial. Figure 10.1 is a picture of Vic as he appeared at the time of his ANL seminar.

I didn't contact Vic at all until 2009 at the time I started writing my paper for Dimitri's Festschrift and which forms the outline of this book [2]. Vic has never bothered to write up a history of RELAP5. Therefore, I had to rely on material sent to me by him and his record notebooks which I copied. I also had to rely on material sent to me by Larry Ybarrondo, Charlie, and Dan Hughes, as well as that gleaned from reports and journal publications to piece together a brief summary history of RELAP5 for this chapter.

As discussed in Sect. 7.5, there was a meeting of Vic and Charlie with Tong, members of the AEC RSR and Regulatory and others on June 28, 1974, in Germantown called the Advanced Code (SLOOP) status review meeting. The material pertaining to RELAP5 is now reviewed for the reader because of its historical significance. Before this meeting took place, a May 8 letter from Tong which was passed on to Vic, mentions using RELAP5 as an intermediate step between the existing code (i.e., RELAP4) and the advanced system code (i.e., SLOOP) some of which modules will be developed elsewhere. This is the earliest recorded mention of RELAP5 that I can find. Then it was at this meeting that the very first mention of RELAP5 is made in Vic's record notebook. Some of the notes of this meeting are in Charlie's handwriting which differs significantly from Vic's. Fabic talked about long-range planning indicating that starting in June 1975 RELAP4 would be phased out, and RELAP5 would be phased in to be completed by December 1976 at which time there is a reference to RST starting. There is no indication as to what RST stands for—Reactor Safety Transient?

Charlie completely left the SLOOP code effort in 1975. When he returned to EG&G, Idaho Inc. in 1980, he became Manager of the LOFT Program Division. Vic stayed on as Manager of the Analytical Model Development Branch for a short while. He stepped down shortly before the SLOOP code imploded. Even though the SLOOP code project failed, the groundwork and experience gained during its aborted three and one-half year development would prove to be invaluable to Vic who, together with Dick Wagner and John Trapp, would initiate the development of the RELAP5 code which it turns out became a success used throughout the world.

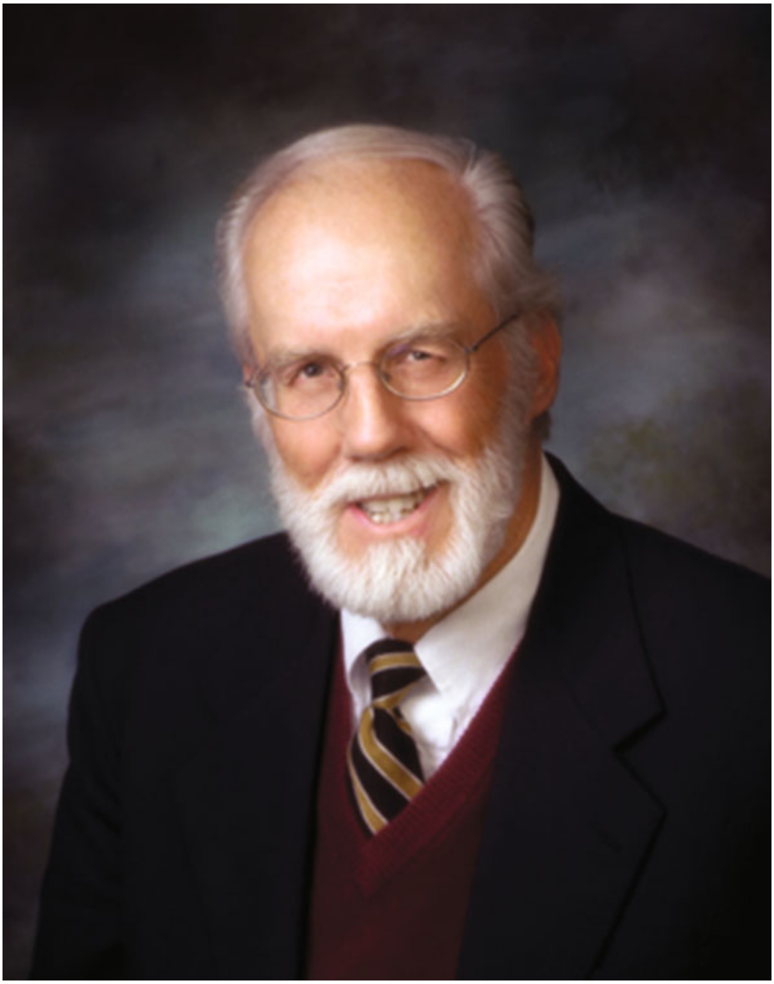

Fig. 10.1 Victor H. Ransom father of the RELAP5 code

But how did it really start? Nobody, not even Vic knew the real story. The major success of the SLOOP code was the discovery of the existence of complex characteristics for the one-dimensional two-phase two-fluid model as documented extensively in Chaps. 6, 7, and 8.

With the change of contractors from ANC to EG&G Idaho, Inc. in 1976 and subsequent reorganization to form the Water Reactor Safety Organization, Larry rose from Manager of the LOFT Division, replaced by Charlie, to become the Associate General Manager of Nuclear Technology. In this powerful position, he had jurisdiction over the LOFT experimental and analytical programs, including the overall computer code development and technical support programs for the NRC.

Since the time he became Manager of the LOFT Program Division in 1973, he had not really been in very close cognizance of what had gone on during the SLOOP code development. So, some time after the SLOOP code imploded, he suggested at one of his monthly staff meetings that it was time for a complete rewrite of RELAP4 to produce a completely new code using an improved equation set and that he would be receptive to receiving such a proposal. Shortly thereafter Vic Ransom and Dick Wagner come forward with a proposal which the three of them discussed. The proposal appeared attractive to Larry. Vic would start over with a completely new equation set and modern programming would be provided by Dick Wagner. Vic changed the name of this proposed code development from SLOOP to RELAP5. Larry considered Vic and Dick proven professionals. But just why did Larry have such confidence in these two individuals? First of all, he knew Dick from the time when Larry joined NRTS in July 1967 and had worked with him closely during the development of the RELAP series of codes. Larry says that Dick was one of the original authors of the RELAPSE-1 [3] (originally called RELAPSE) and CONTEMPT [4] computer programs. He was a fine physicist and a superb programmer. He had always exceeded or met his commitments to Larry. Vic Ransom had been recommended to Larry by Hal Campen, Director of Engineering at Aerojet Nuclear in 1973. Larry followed up on Hal's recommendation and hired Vic on April 24, 1973, and considered him a success at all the tasks assigned to him. Vic was a theoretician and Dick was a consummate systems programmer. He had complete confidence that they both would be up to the task to produce the new code and that they would probably produce more than they promised. Having Dick Wagner to work with Vic was a real plus. He should have worked on the SLOOP code effort but he was busy in programming efforts for the RELAP4 code [5] and its subsequent revisions, or MODS, which were under development at the same time [6].

As Larry recalls that the budget Vic and Dick proposed to produce the first working version of the new code was about $50,000. John Trapp, who received his Ph.D. in Continuum Mechanics from the University of California, Berkeley, made a significant contributions to the now defunct SLOOP code effort and had stayed behind effort, was also to be part of the new code development. They estimated that the initial version of RELAP5 was to be drafted over a several months time frame. However, Larry was confronted with a serious decision. Larry's annual budget for the Nuclear Technology organization which he managed was on the order of $158 million. As most people who have worked with government funds know, government funds come in different "colors" which is to say that some funds may only be used for specific purposes such as equipment and construction and may not be used for any other purpose; it is illegal to do so. Larry was sure that if he requested $50,000 from the NRC for this proposed code development effort, the answer would be a definite no. This was because members of the NRC were in effect encouraging members of the EG&G, Idaho Analytical Group to leave for LANL where the TRAC advanced code development effort was under development [7]. They were also leaving for the spin-off companies Energy Incorporated started by Chuck Rice and Intermountain Technologies, Inc. started by George Brockett. As discussed in Chap. 7, this kind of thing had been going on for some time when the NRC (think Fabic and Tong) began moving analysis development work from ANC with a concomitant decrease in funding to Los Alamos National Laboratory where they felt that there was superior code development capability. They were also demoralizing the ANC code developers with heavy negative criticism of their work.

Larry discussed the matter of the $50,000 for the RELAP5 code development proposal with his supervisor Ron Kiehn, Manager of EG&G Idaho, Inc. He agreed with Larry's judgment to withdraw the funds from accounts he would select. Larry had a charge account created. The funds were then transferred, and the initial RELAP5 effort commenced. Neither Vic nor Dick nor anyone else had *any* knowledge of where the funds were coming from or the amount used. That was for their protection. Fortunately for Larry, no one bothered to ask where the funds came from.

The RELAP5 project apparently started in 1975 shortly after Larry set up the charge account for Vic, Dick, and John Trapp to begin development on it. The best I can do to trace its early development is to refer to the report by Jackson et al. prepared for the Nuclear Reactor Safety Heat Transfer 1980 Summer School and International Seminar, August 25–September 5, 1980 [6], and to Vic's sporadic entries in his record notebooks. As early as June 1976 Trapp and Ransom issued a report on the field equations [8]. Around August 5, 1976, there are a couple of entries in Vic's record notebooks concerning writing up a blurb for RELAP5 and then a discussion with Tong and Fabic about having the code run some preliminary checkout problems by June 30. In late 1976, Trapp and Ransom issued a progress report on the hydrodynamic model [9]. On February 4, 1977, there is an entry in Vic's record notebook for a staff meeting with Larry present concerning the development of specifications for the RELAP5 document. There is a six-page entry for a March 24 and meeting of Vic at LASL discussing the SOLA-PLOOP code with Tony Hirt, Tom Oliphant, Dennis Liles, Bill Rivard, and Jack Travis. This code was scheduled to be released in October. In 1977, there is a presentation of RELAP5 code development and results at the Fifth Water Reactor Safety Research Information Meeting [10]. Then there follow two reports in 1977 and 1978 on abrupt area changes and branching [11] and choking model [12]. In January 1978, there appears the RELAP5 PILOT [13] code and in May 1979 there appears documentation of the first operational release of RELAP5 [14]. Jackson et al. [6] refer to this as RELAP5/MOD0 which was available from the National Energy Software Center and present its status, model description, and example calculations. The draft of RELAP5/MOD1 appears in 1980 [1]. Trapp documented the evaluation of RELAP5/MOD0 together with comparisons to RETRAN-02 and TRAC-P1A [15].

Recently, Larry discussed the origins of RELAP5 with Roger Mattson, former Director of the Division of Systems Safety in the Office of Nuclear Reactor Regulation at the NRC. He related the following information. Thomas E. Murley who was head of the NRC Division of Reactor Safety Research in which Tong and Fabic worked was not pleased when he found out about the RELAP5 code. Why? As Larry understood it, Murley had been trying to transfer the code work at EG&G

Idaho, Inc. to the LASL Group-T-3. This reinforces the suspicions that the SLOOP code members concluded early on. A quote attributed to Murley was something like, "The folks at EG&G are not good enough to carry the jock straps of the LASL guys." Larry wasn't sure if that was an exact quote but it is quite descriptive capturing the essence of what Murley said. However, Roger Mattson, who was Director of the NRC Division of Systems Safety in the Office of Nuclear Reactor Regulation Licensing was the source of funding and the customer for the EG&G Idaho, Inc. work that the NRC Division of Reactor Safety Research was monitoring. Murley asked Roger to shut off the funding. Roger refused saying, "Let EG&G and LANL compete, NRC Licensing wants the best code for licensing." RELAP5 was an instant success. It was a seminal, state-of-art product even at its initial stage of development. An uproar occurred as soon as it was clear that RELAP5 was accurate, faster, and easier to use than any other existing nuclear systems computer code.

RELAP5 went through several major versions over the next roughly 15 years after the release of RELAP5/MOD0 in 1979: MOD1 in 1980 [1], MOD2 in 1985 [16], and RELAP5/MOD3 in 1995 [17]. Development work ended formally when the NRC sponsored development of RELAP5 was transferred to SCIENTECH, Inc. for maintenance and release of RELAP5/MOD3.3. SCIENTECH, Inc. was an employee-owned company founded in the fall of 1982, when Larry left EG&G Idaho, Inc. and started the company with his wife Mary Ann. Roger Mattson became a principal owner several years later. Larry built up and managed the company for 17 years. Subsequently the project was transferred to the Innovative Systems Software in Idaho Falls, Idaho. Their Web site advertises their roles of RELAP5 and RELAP/SCDARSIM in Nuclear Safety and Research Reactor Safety [18]. Larry recently was told by Jim Myer, an ex-NRC employee, that RELAP5 is used all over the world. He noted that it would be difficult to license a nuclear power plant without using the data from the INL tests and RELAP5. The last word comes from Vic Ransom. His personal belief is that the RELAP5 type of code is adequate for safety work when the uncertainties are properly accounted for using statistical methods. Because of the broad spectrum of uncertainties, little improvement in safety margin can be obtained by improvements in the one-dimensional two-phase model alone.

According to the NRC Web site it has been working for some time on merging TRAC with RELAP5 to produce what they refer to as TRACE (<u>T</u>RAC/<u>R</u>ELAP <u>A</u>dvanced <u>C</u>omputational <u>E</u>ngine. [19, 20]. TRACE is meant to be a modernized thermal hydraulics code designed to consolidate and extend the capabilities of NRC's legacy safety codes TRAC and RELAP5. It is claimed to be able to analyze large- and small-break LOCAs and system transients in both pressurized and boiling water reactors (PWRs and BWRs). The capability exists to model thermal hydraulic phenomena in both one-dimensional and three-dimensional space. This is the NRC's flagship thermal hydraulics analysis tool. Although RELAP5 still enjoys widespread use in the nuclear community, active maintenance will be phased out as usage of TRACE grows. For more information on the TRAC code, the reader is referred to Jackson et al. [6].

Lopez de Bertodano et al. Chap. 5 [21] briefly discusses the RELAP5/MOD3.3 two-fluid models and compares them with those in the TRACE code. Martin Lopez de Bertodano is at the School of Nuclear Engineering, Purdue University, William Fullmer, formerly at Purdue University as now at the University of Colorado, Boulder, Alejandro Clausse is at the University of Central Buenos Aires & CONICET, National Energy Commission, Buenos Aires, and Vic Ransom is Professor Emeritus at the School of Nuclear Engineering, Purdue University. Although I didn't explicitly mention it, RELAP5 solves the one-dimensional two-fluid two-phase equations while TRACE, like TRAC, solves the three-dimensional equations. RELAP5 and TRACE have the volume fraction outside the pressure gradient in the momentum equations. RELAP5/MOD3.3 has an incomplete added mass equation dropping the spatial derivatives [21], while TRACE does not have the added mass term. As far as I can determine, the full added mass term was included in RELAP5/MOD1 [1], RELAP5/MOD2 [16] and all the way up to RELAP5/MOD3 [17]. No matter, the equations are not completely hyperbolic since there are regions where the characteristics become complex [21]. A velocity difference equation is employed which I developed for use in RELAP4 with slip [22], subsequently incorporated into RETRAN [23], and published in 1979 [24]. The authors of this book had an opportunity to expand upon the RELAP5 history and attributes but failed to do so.

RELAP-7 (What happened to RELAP-6?) is a new project started in 2012 at the Idaho National Laboratory (INL) [25]. The RELAP-7 code is supposed to be the next-generation nuclear reactor system safety analysis code. The overall design goal of RELAP-7 claims to build upon 30 years of advancements in computer architecture, software design, numerical methods, and physical models. The end result is envisioned to be a reactor systems analysis capability that retains and improves upon RELAP5 and TRACE. I know even less about the reason for developing RELAP5-3D and the reason for its development. There is a RELAP5-3D International RELAP5 Users Group (Web site http://www4vip.inl.gov/relap5/irug.htm). There was a RELAP5-3D Users Seminar in Idaho Falls in 2008 and a more recent one in Salt Lake City. It seems to me that there is a lot of redundancy in the development of these hybrid codes.

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Chapter 11
DOE Starts Code Development at Systems, Science and Software and JAYCOR to Address the Energy Crisis Caused by the Oil Embargos

Spurred on by the lingering effects of the Arab oil embargo in 1973–74, ERDA funded two institutions to model fluidized-bed gasifiers. The first was Systems, Science and Software (S^3 or S cubed) and then JAYCOR. In Chap. 9, I briefly discussed my interaction with S^3 located in La Jolla California while I was at EI. Dr. M.F. Scharff was the project manager in 1975 during the first year of the ERDA contract titled Computer Modeling of Coal Gasification Reactors. However, he left for JAYCOR during the first year of the contract for another consulting company located in San Diego. Dr. Thomas Blake took over his position. The contract was funded at $1,270,000 for 3 years. The objective of first year was to establish a firm theoretical description of the multiphase hydrodynamics and chemical behavior of high-BTU gasification reactors through the development of one- and two-dimensional computer models. In the second and third years, the models were to be expanded to apply for low-BTU and entrained flow gasifiers. The model which was adopted is based on Jackson's [1] which neglects gas momentum effects which are important for high-speed jets entering fluidized beds. In place of a full momentum gas balance, Darcy's law is used and the solids momentum balance includes a solid-phase viscosity in the viscous terms with adjustable parameters and an expression for the solids pressure [2–4]. Dimitri's experience shows that such stresses can be neglected as a first approximation [5].

This model was the first to produce realistic bubble formation created by continuous flow through a gas jet into the bed without the necessity of postulating a "bubble phase" [3, 4]. The computation was done for inlet gas jets separated by 32 cm into a slumped bed initially 32 cm high. The bed consisted of glass beads 860 micron in diameter having a density of 3 g/cm^3. Three cases, A, B, and C, were run with gas jet velocities of 295, 328, and 361 cm/s, respectively, to illustrate bubble formation and decay in decay for an insufficiently fluidized bed (Case A), bubble formation growth, bursting into the freeboard, and collapsing (Case B) and jet penetration resembling a spouted bed (Case C). No comparisons to experiments

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were made. The contract was extended for a fourth year which started in October 1978 by which time the entrained bed gasification reactor model was developed [6]. The third year of the contract would have ended in June 1978. The gap of 3 months may have been involved with renegotiating the contract. Comparisons with data from the IGT bench scale and U-GAS reactors and Westinghouse agglomerating combustor/gasifier were made. A four-volume final report was issued in 1981 [7]. Included was a user's manual for the fluidized-bed gasifier code, which was named CHEMFLUB (Vol. 3), and the EF (Entrained Flow) computer model (Vol. 4). To my mind, these two volumes do not much resemble user friendly code manuals. Work was then terminated on the S^3 codes. This might have been the reason that a contract was given by the DOE to the BDM Corporation in McLean, Virginia, to analyze the CHEMFLUB code documented in a two-volume report [8]. This included the mathematical formulation, closure equations, chemistry models, and solution algorithms. Both of these volumes authored by BDM are shoddily done with barely visible handwritten equations in Volume *I* and tables of computer output instead of graphics in Volume 2. I would consider this documentation next to useless. LANL evaluated the S^3 entrained flow gasifier code and identified enhancements needed for engineering of commercial process [9].

After the conclusion of the CHEMFLUB code development at S^3, the second DOE fluidized-bed computer code called FLAG was developed by JAYCOR [10]. Its origin might have started as a competitor to S^3 since M.F. Scharff had left S^3 to join JAYCOR. FLAG modeled the void fraction from the number of particles in a unit cell obviating the need to write an equation of motion for the solid phase. The single particle equation of motion was used to compute the trajectories for a select group of fluidized-bed particles representing the many which exist in a control volume. Thus, this select group of particles can be characterized as "pseudo-particles." All frictional interaction between particles was neglected as were the so-called added mass inertial forces, and so interaction between different size particles will result in an incorrect prediction of segregation. So, the FLAG code was even less mechanistic than the CHEMFLUB code. The lifespan of the FLAG code development was quite short. It was subsequently documented in another DOE contract to the BDM Corporation [11]. Smoot [12] and Dimitri, in his D.Q. Kern Award Lecture [13], reviewed the history of these efforts to which the reader is referred. These computer codes were installed on the Morgantown Energy Technology Center (METC) computer and evaluated by West Virginia University (WVU) to identify their merits and demerits. The DOE Technology Status Report for 1986 reported that "WVU has found that CHEMFLUB, a fluidized-bed model, fails to simulate most of the major hydrodynamic fluidization characteristics and suggested the modifications of the pressure drop equation in the CHEMFLUB model" [14]. It turns out that that METC found both CHEMFLUB and FLAG to be failures in spite of the millions of dollars spent to develop them. The story of the DOE effort to develop a working fluidized-bed computer model will be discussed further in Chaps. 12 and 13.

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Chapter 12
IIT Code Begins Using Los Alamos' K-FIX Code

I ended Chap. 9 with my leaving Energy Incorporated and Idaho on June 17, 1977 (it turns out permanently), for employment at Lawrence Livermore Laboratory (LLL) in the Underground Coal Gasification (UCG) project. To the outside world, my switch from nuclear energy to fossil energy would seem incongruous but to me it was natural. The thread was the application of my understanding of the fundamentals of multiphase theory. Dimitri encouraged me to join saying that there were a lot of multiphase problems waiting to be solved. After my worldly goods were loaded into the moving van, I drove my car (an Audi) from Idaho to California on the weekend together with my bicycle firmly attached on a rack secured from the trunk of my car. So, I bid adieu to Idaho and was off to California. Upon arrival, I checked into a motel in Livermore. Then I contacted the real estate agent in Livermore whom I had talked with via telephone and mail before I left Idaho. We made a tour of Livermore, looked at a few houses in various sections of the city. Then we set up a schedule to look at houses for sale in the price range I decided upon. The real estate agent and I went house hunting during the weekend. I found a house to my liking and budget located just a few miles from the laboratory. I was disappointed that none of the houses we looked at had basements, but the house I decided upon had four bedrooms in which I could distribute my worldly goods upon arrival of the moving van. During the time I was at LLL, I would frequently bicycle the short distance to the laboratory.

On June 20, 1977, I checked into the personnel office. After taking care of the necessary paperwork, I received my badge which was necessary for entering the laboratory. I was then greeted by Dr. Terry Galloway who gave me a short tour of some facilities walking on the way to our UCG offices located in a trailer complex. One of these facilities was, as I recall, the mammoth Tandem Mirror Fusion facility. I had my "Q" clearance renewed beforehand, and so I didn't have to spend any time in the uncleared bullpen area until it would have been approved. The UCG team was housed in a complex of trailers connected together just east of a building where the small oil shale retorting experiments were performed. The UCG program was under the leadership of Douglas R. Stephens who greeted me. The underground oil

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shale retorting program was housed in another trailer complex further west. The geothermal program trailers were close by. These trailers were located inside the perimeter fence through which one would enter through the security guard post from the parking lot by showing your badge. My office was in one of the trailers with a window facing this building. These trailers were none too sturdy. When one walked around between offices, a booming sound would emanate from the floor. There was a satellite computer terminal in this trailer which was connected to the LLL computers. There was also a large oil shale retort located outside north of the UCG trailer complex. Bob Cena, Dave Gregg, Terry Galloway and myself constituted the modeling group for the UCG project under our immediate supervisor Charles Thorsness, who was called Chuck by everyone. Chuck's supervisor was Rudy Rozsa who might have been related to the famous Hungarian composer Miklos Rozsa (I never asked him). Delores Olness was the person in charge of translating the Russian UCG literature and assembling the quarterly progress reports. I was given pretty much free reign to work on just about any aspect of UCG that interested me. Dave Gregg was the group's free spirit who seemed to work on whatever pleased him. I would spend many happy hours bouncing ideas off of him. More about Dave Gregg is given later.

The field tests for the UCG project were located near Gillette, Wyoming. Douglas Stephens and Richard Hill were the leaders of these field tests and they were out of the office for extended periods of time. The experiments were complex and time-consuming to set up. The runs themselves would take many weeks apiece. Chuck Thorsness was the one primarily responsible for data reduction and interpretation of the field tests, and Bob Cena would assist him. In truth, my impression was that no one really knew what was going on underground as the coal seam was being gasified. Sometimes no coal gas would exit the production well. Shortly after I started the UCG project, Bill Aiman was hired to carry out laboratory experiments to throw light on the mechanisms of just how the coal was being gasified underground. His background was as an experimentalist from General Motors studying internal combustion engines. He would carry out his experiments outside of the trailers gasifying coal monoliths brought in from Gillette encased in 55-gallon drums. These coal monoliths were saturated with water which came from the aquifer. Bill would bore a channel through each of these drums and ignited the coal to simulate what was occurring underground. He studied both forward and reverse combustion as I remember. I still have a photograph of Bill performing one of these experiments.

I used my imagination to start applying multiphase flow to explain some of the things which Bill was finding from his experiments. I decided to model drying because in my opinion, one cannot burn coal until it dries out. The coal seams being gasified in Gillette, Wyoming, were always infiltrated with water from nearby aquifers. Water snuffing out the burn was the explanation for the "zero-BTU" gas sometimes produced. Consequently, I developed a model for drying [1, 2] which was used to explain the laboratory experiments [3] and which would be used in conjunction in the model used to interpret the UCG field tests [4]. One field test injected pulses of helium into the coal seam during a gasification test to act as a tracer. The idea was to determine the active void volume, i.e., the size of the burned-out coal seam cavity. I spent some time to understand dispersion theory and then to apply it to interpret the experiment [5]. Later after I went to IGT in 1979, I was lucky enough to take with me a small contract with LLL to do further research on two-phase drying theory [6]. I used Green's functions to develop a simple model to interpret the thermocouple data taken during the field tests [7]. The conclusion was that they had to be extremely close to the burn front to register an appreciable response

Rudy Rozsa decided that I could be of some help to the in situ oil shale project and so I started to work half time on it. Bob Braun and Ray Chin were the developers of a one-dimensional oil shale retorting model. I started to study the documentation and soon found some deficiencies, the most serious of which was the treatment of the heat capacity. It was outside the derivative of temperature in the energy equation. I alerted them and soon a meeting took place. I explained why the heat capacity needed to be inside with the derivative of the temperature. I convinced them, and after they modified their computer program, comparisons with experiment improved. After that, I was trusted by the leaders of the program, Art Lewis and Al Rothman. After that, I applied myself to improving their model using concepts from multiphase theory. What was missing in the oil shale retorting model was the production of a liquid mist which was produced as the major product. The retorting model lumped all of the product into "gas." I collaborated with Dimitri on developing a model for the oil mist production [8] and another to explain anomalous pressure oscillations [9] and with Ray Chin on plugging of oil shale by the mist [10]. I also worked with Terry Galloway who was appointed to head the large retort experiments. This retort as I mentioned above had to be outside of the laboratory where the small oil shale retort experiments were performed since it was 20 ft (6.1 m) high and 3 ft (0.91 m) in diameter. The first (and only) experimental run produced many anomalous results which I decided I would try to explain. I applied dispersion theory, a lot of thought, and then simulated the experiment using COBRA, a computer program developed for nuclear reactor core analysis that Bob Cena had worked on at PNL and brought to LLL [11]. I also worked with Terry to interpret the large retort experiment [12]. Later I developed an extended multiphase theory to describe flow in fissured media having a wide size distribution [13].

Before beginning the story about how the IIT code started, I have to relate an experience concerning an episode emanating from my nuclear career. In 1975, Dimitri sent me a paper to review for his AIChE sessions for the 15th National Heat Transfer Conference held in San Francisco. It was manuscript titled Numerical Calculation of Two-Phase Flows by J.R. Travis, F.H. Harlow, and A.A. Amsden. I spent a great deal of time reviewing the manuscript and concentrated my remarks in the section Drift-Flux Approximation. I returned the review to Dimitri in February. I gave it a fair rating stating that it was acceptable for presentation and could be acceptable for publication with revisions. This manuscript was issued as a LASL report later that year [14]. I considered the matter ended. In 1979 when I was at LLL, I ran across this same paper published in 1976 with minor revisions [15]. I decided to send a Letter to the Editor, Dixon Callihan, the same editor to whom

I sent the characteristics paper manuscript (see Sect. 8.3), concerning the section on the "Drift-Flux Approximation." I mailed it on March 6 and to my surprise this set off a minor firestorm. My letter to the editor was published [16] followed directly by a reply by the authors [17]. Then I received a letter from Dixon Callihan on November 2 transmitting remarks from Tom Porsching, of the FLASH numerical scheme fame (see Chap. 9), on my letter to the editor. I was really concerned that I may have made some serious errors in my letter, so I contacted Ray Chin who was working in the oil shale program, to discuss the situation and to help me to write a reply. I met with Ray and his friend Louis Thigpen who worked in the seismology program. Ray was a distinguished mathematician and at the time was one of the editors of the Journal of Computational Physics. They were very helpful in elucidating the mathematical consequences of the Drift-Flux Approximation made by Travis et al. I mailed the reply which was published following Porsching's [18, 19] and that ended the dialog. I should mention that Ray and Louis became good friends, and on Fridays after work, we would retire to the Matador Lounge, a popular watering hole for LLL employees, a short distance from the laboratory. Then we would drive to Oakland for Chinese food at Ray's favorite restaurant, the Joy Luck and more drinks.

12.1 K-FIX Code Obtained from Bill Rivard to Start IIT Code

The idea for the IIT and FLUFIX codes really began in 1977–1978. As I mentioned earlier, Dimitri came out to LLL to consult for the UCG program and later for the oil shale program. He helped Terry Galloway and myself to develop a step-by-step building-block hydrodynamic computer modeling approach for understanding the hydrodynamics of fluidized beds, coupled to validation experiments [20]. This is when I made Dimitri aware of the K-FIX code [21]. As I discussed in Chap. 9, I had been involved at EI when I was a consultant for EG&G Idaho, Inc. in a project using K-FIX to model the two-dimensional flow in the cold leg of the LOFT blowdown experiments. The LLL report formed the basis of Dimitri's response to a DOE (established as the successor to ERDA on October 1, 1977) University Programs Request for Proposal (RFP) in 1977. Dimitri proposed in his response to the DOE to use the two-dimensional K-FIX code to perform the calculations for his grant and, in anticipation of his being successful in obtaining funding, asked me to obtain it from LASL. The anticipated plan would be to modify K-FIX so that it could realistically simulate a fluidized bed in two dimensions. At this point, I remind the reader of DOE's efforts around this time to produce fluidized-bed gasification codes at S^3 and JAYCOR in response to the Arab oil embargo as described in Chap. 11.

So in September 1977, I called Bill Rivard at LASL, primary author of the K-FIX computer program asking whether it was possible he could send me a copy of the code. I told him that Margaret Butler, who was in charge of the Argonne

Code Center at the time, had informed me that it had not yet been installed. He agreed to send it and so I sent him a tape with instructions on how to copy the code onto it. I also asked Bill for updates to correct any errors which may have been found. He promptly sent me the tape back containing K-FIX. In his cover letter, he stated that there were additional statements on the tape required to run the sample problem described in the code manual [21]. He went on to say that this prerelease version of the code was a card-by-card copy of the LASL FORTRAN source deck. This may or may not have been identical to the version sent to the Argonne Code Center. He concluded his letter with "Good computing." I had the tape read at the LLL computer facility on one of their computers. This went flawlessly, and I subsequently proceeded to compile the K-FIX using the LLL UPDATE and SLOPE simulator software to keep a clear record of any changes that might be made to the code. This activity was under the guise of applying K-FIX to (now hold on) solar retorting of oil shale and gasification of coal in a solar fluidized bed. Dave Gregg had started a big stir when he decided that if solar energy were used instead of air, yields and quality of the product would be much improved. He called this his "Solar Synfuels Program" which was reported in Life magazine. He received funds to construct a retort at LLL into which was placed a packed bed of either oil shale or coal. The retort contained a window through which the solar radiation would enter. The apparatus was transported to the White Sands Proving ground and assembled atop a focused solar energy platform to demonstrate feasibility, and it worked for both gasifying coal and retorting oil shale. After this initial exercise, I didn't really do anything more with the K-FIX code until Dimitri got his grant. I fiddled around and developed a conceptual model for this solar fluidized-bed gasifier for both agglomerating and non-agglomerating coals as shown in Fig. 12.1.

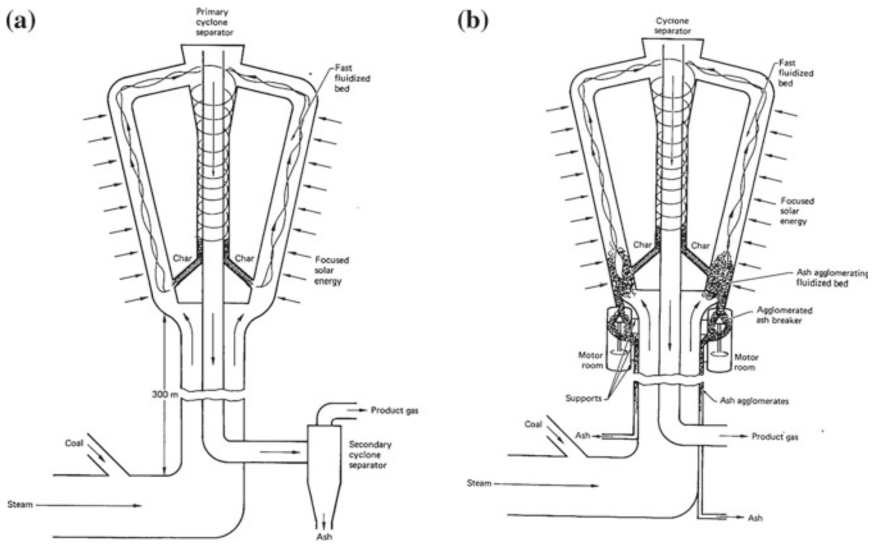

Fig. 12.1 Solar fluidized-bed gasifier models. **(a)** Non-agglomerating **(b)** Agglomerating

A two-year grant to study solids circulation around a jet in a thin "two-dimensional" rectangular fluidized bed was awarded to Dimitri in September 1978, thus initiating his 40-year research into fluidization. To accomplish the objectives of his proposal would require transforming K-FIX from a gas–liquid computer program, developed to simulate the hypothetical core disassembly accident (HDCA) for sodium-cooled fast breeder nuclear reactors, to a gas–solids (or, more generally, a fluid–solids) computer program using interfacial drag models specified by him. A fluidized-bed experiment was constructed and run at IIT in order to validate the modified computer program. A traveling gamma-ray densitometer would measure the time-averaged gas-phase volume fraction. This validation experiment would be the key to success missing in the failures of the S^3 and JAYCOR computer codes. Dimitri assigned his Ph.D. student Bozorg Ettehadieh to the project. Bozorg spent the early months of 1979 constructing and shaking down the experimental fluidized-bed apparatus. Dimitri had Bozorg write up the gas–solids drag function model which he sent to me. It was based on the well-known Ergun equation used for fluid flow in porous media for a gas-phase volume fraction less than 0.8 and a modification of the single sphere drag function for a gas-phase volume fraction greater than 0.8 [22]. Joe Ching, with whom I had worked with at EI, joined the Nuclear Engineering Department at the University of California, Berkeley (UCB) at precisely the same time I joined LLL. Joe and his fraternal twin brother Hugh would help me to purchase a ten-unit apartment in Berkeley. Hugh was a savvy real estate person with a Ph.D. in nuclear engineering as was his brother Joe. Hugh was able to use my collateral to help his brother purchase a twenty-plus-unit apartment building in Berkeley not far from mine. That is the reason I alluded to Joe and me as "partners in crime" at the end of Chap. 9.

Joe had access to the UCB Nuclear Engineering Department and Lawrence Berkeley Laboratory (LBL) mainframe computer, and since he was a computer code expert, he ran a workshop for the department's students. He already had K-FIX, TRAC and many other nuclear computer codes available for use in this workshop. In May 1979, I sent material to Dimitri briefly describing the K-FIX and TRAC codes to help him decide which one to use. We briefly considered using the TRAC code but we found that it was too complex, and besides I had no experience with it. Dimitri and I decided that it would be all together cleaner to have Joe do the computer work for his grant since he was much more experienced than I. Therefore, it was to Joe that Dimitri gave a small contract in July 1979 to program the interfacial drag function into the K-FIX code, add the new variables needed, and compile it. He accomplished these crucial tasks and then transferred the modified K-FIX code back to me at LLL. I compiled the K-FIX code on one of the unclassified CDC computers at LLL. Now I could begin exercising it to simulate a high-speed gas jet injected into a fluidized bed under the guise of modeling my solar-powered fluidized-bed idea for coal gasification. The code seemed to produce reasonable results. Without resources for computer graphics visualization, I drew the bubble formation and solids circulation patterns by hand. Figure 12.2 shows a plot of the solids and gas velocity vectors, gas volume fractions (porosities), and an

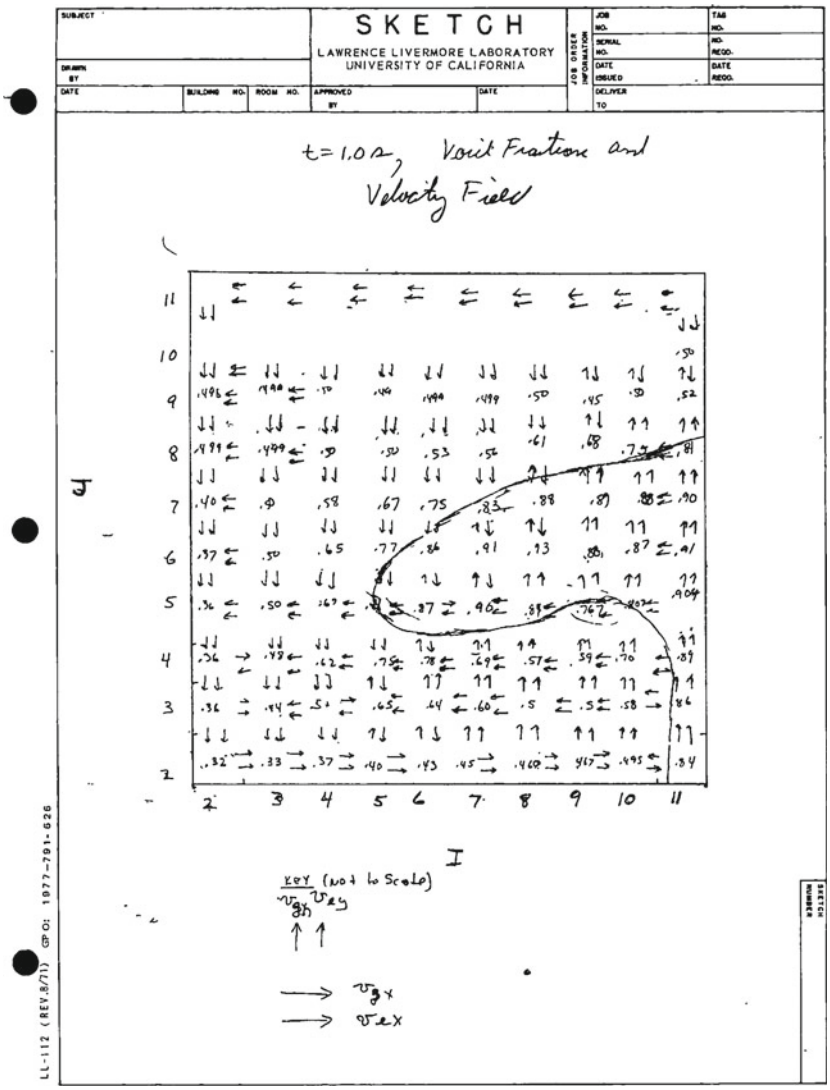

Fig. 12.2 Gas and solids velocity vectors and gas volume fractions computed from the modified K-FIX computer program

estimate of the bubble shape at a gas volume fraction = 0.8 at a transient time of 1.0 s. Figure 12.3 shows a plot of the estimated solids circulation pattern also at 1.0 s. I really believe these were the first computations to produce realistic results for bubble formation in a fluidized bed.

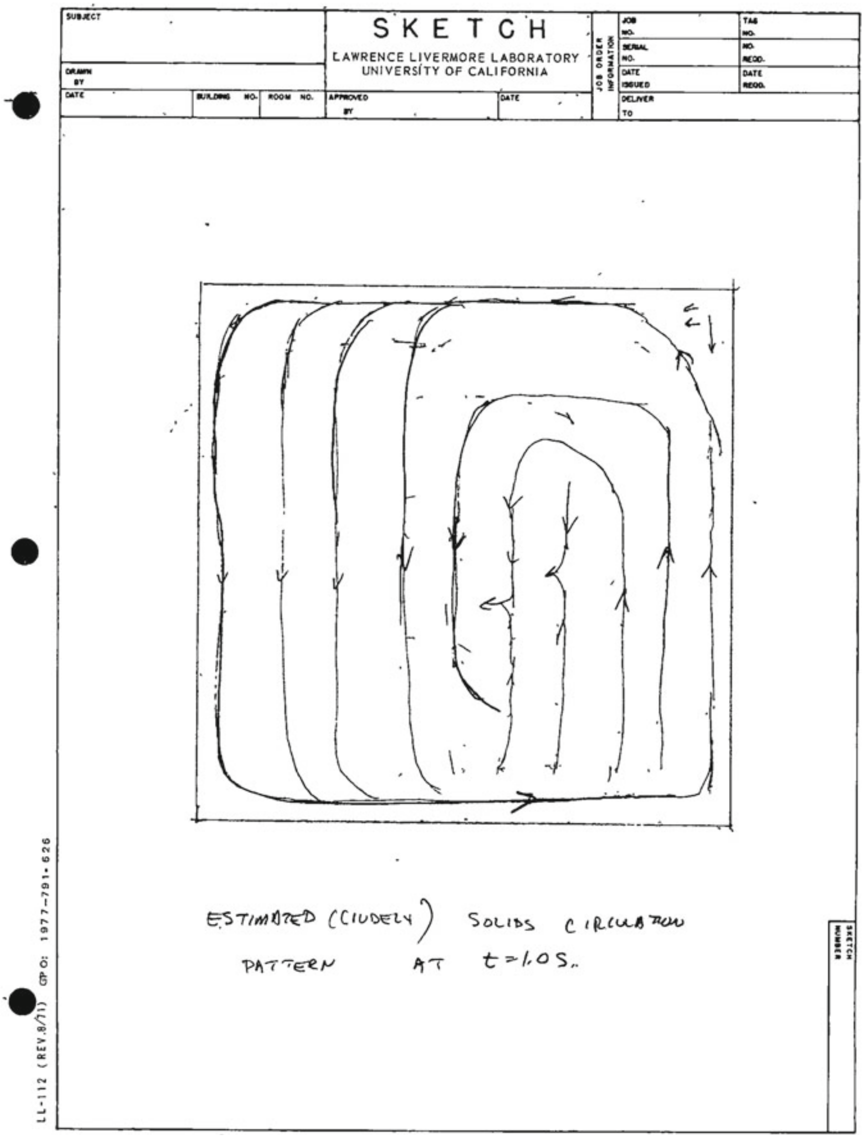

Fig. 12.3 Estimated solids circulation patter computed from the modified K-FIX computer code

I prepared a long handwritten report summarizing what had been accomplished which I sent to Dimitri. It was titled Two-Dimensional Computer Modeling of Fluidized Beds by myself and Joe Ching. I include the first few sentences below.

> The transient two-dimensional two-phase computer program K-FIX [21] has been used to simulate the start-up of a fluidized bed from an initially quiescent state. The major objective

> was to determine the computer code's capability to predict solids circulation in a two-dimensional cold fluidized bed using as a starting point some of the experimental data of Yang and Keairns [23]. The computer code was changed and modified only to the extent that this simulation could be performed and in a reasonable amount of computer time with unmodified field equations. There remain code deficiencies and possible outright "bugs" in this semiproduction public version of K-FIX. They will be reviewed in a later section.

I included hand-drawn figures prepared from the computer printout.

Then Bozorg Ettehadieh flew out from IIT to Berkeley to work with Joe Ching and myself so that he could become familiar with running the modified K-FIX fluidized-bed code. As I recall he stayed at Joe's apartment building. After this indoctrination period, Bozorg returned to IIT and installed the code on the Chemical Engineering Department's Prime computer. He thus became the first student of Dimitri's or anyone else to model a two-dimensional fluidized-bed transient.

In December 1979, I left LLL and joined the IIT Department of Gas Technology housed in IGT. One reason I did this was I reasoned that it would allow me to work more closely with Dimitri and his Ph.D. student Bozorg and to continue to offer him informal advice. However, I was not to stay at IGT very long. More about this decision is given as follows.

Following Dimitri's first DOE grant, there followed a two-year grant by the Gas Research Institute (now the Gas Technology Institute, GTI) in January 1980. Then there was a three-year NSF grant in 1982 and a two-year contract with Westinghouse Electric Corp. (Synthetic Fuels Division; later KRW Energy Systems, Inc. and now defunct) in 1981. These grants made it possible for Dimitri to continue implementing the step-by-step approach and to allow the early research to continue for nearly 40 years. The primary focus early on was synfuels production using fluidized-bed gasifiers since this was in the era of the continuing energy shortage caused by the Arab oil embargo. Things started to become worse than the 1973 Arab oil embargo early in 1979 with oil prices increasing from less than $5 per barrel to $15 per barrel, which was bad enough, escalating to nearly $40 per barrel by 1981. Progress was slow because computer running times were extremely long on IIT's Prime computer, and the cost of more powerful mainframe computer time was prohibitive. I clearly remember visiting Bozorg in the laboratory where his computer terminal was located. About once every minute, the time step would advance and print out. Bozorg received his Ph.D. in May 1982. The first paper documenting this simulation of the thin "two-dimensional" fluidized bed with a central jet was published in 1983 [22]. Lacking graphics, he used the same manually produced visualizations of bubble formation and solids circulation as I did. Madhava Syamlal became Dimitri's second Ph.D. student to follow on Bozorg's computer fluidization work [24]. Bozorg stayed on as a postdoctoral fellow for a year assisting Dimitri on a contract from Westinghouse Electric Synthetic Fuels Division near Pittsburgh to model their pilot demonstration unit (PDU) fluidized-bed coal gasification reactor. He was subsequently hired by them in 1983 to work on modeling, analysis, and instrumentation development for their large-scale 10-feet (3.05 m)-diameter 30-feet (9.1 m)-high cold fluidized-bed experimental facility. The Synfuels Division was subsequently acquired by W.M. Kellog Rust Company and became KRW Energy Systems Inc. He worked closely with W.C. Yang who was at the Research and Development Center, Westinghouse Electric Corporation. Before Bozorg left IIT, we collaborated on a paper [25]. The fluidized-bed experimental program at KRW went on for several years but was eventually terminated when the price of oil plummeted in the late 1980s to early 1990s. In 1990, Bozorg joined Rhone-Poulenc Inc. (Rhodia, USA) in Houston, TX:

As I mentioned above, I left LLL in 1979 and joined IGT. In effect, I was replacing Dimitri who had left IGT in 1977 to become Professor in the Chemical Engineering Department at IIT at the invitation of the Chair, Darsh Wasan. The main reason I decided to join IGT as an Associate Professor in the Gas Technology Department was that, in addition to working with Dimitri and Bozorg, I thought it would allow me to collaborate fruitfully with its staff on gasification research. This did not materialize since the IGT staff members were highly protective of their turf and didn't cooperate with the Gas Technology Department faculty. I was able to obtain a small contract with LLL titled Modeling Moisture Dynamics of Coal to do further research on two-phase drying theory. I hired a student to work on the contract for his M. S. thesis which resulted in a peer-reviewed publication [6]. I was assigned to develop a new course called Unconventional Energy Extraction and Conversion and to teach the fluid flow course. Stuart Leipziger, who had replaced Richard Bukacek as Chair, was the one who encouraged me to join the Gas Technology Department. The rest of the full-time faculty consisted of Hamid Arastoopour, a recent graduate student of Dimitri's, and Hisashi Kono, a more mature Japanese gentleman who was primarily an experimentalist with expertise in gasification. I found out that the Gas Technology faculty members were only elected to the IIT faculty. We were in fact only Adjunct Faculty and so were treated as second class citizens. In one of the only meetings that I had with Donald Klass Director of the Education Division, I was informed that I could not do consulting. This was not told to me before I accepted IGT's employment offer. He said "Your mind belongs to IGT." To make it clear to the reader, I was an employee of IGT, not IIT. My paycheck came from IGT as did the benefits. He had a plaque on his wall that said "Research is where the money is." That broke the camel's back, and I decided to make plans to leave. Little did I know at the time that IGT had clandestinely developed a plan to close down the Gas Technology Department. This was discussed back in Chap. 3. Hishashi Kono may have learned of this plan and left for West Virginia University during 1980. If I had stayed, it would have been extremely nasty for me.

I received an offer in late 1980 from Bill Sha at Argonne National Laboratory to work with his group in the Components Technology Division (later the Energy Technology Division) to work on his COMMIX-2 code development project for the NRC. This was the second time he offered me such a position, the first shortly after I joined LLL in 1977 which I declined. Actually this was the third time I had received an offer from ANL. The first was from the Reactor and Safety Analysis Division to work on their fast breeder code development. I went to Energy Incorporated instead. This time I accepted Bill's offer. Zounds, I would now be back in the nuclear industry! I left IGT effective the last working day in February 1981, for a tenure there of just over one calendar year starting in December 1979. Just before I left, I finished writing the review article Multiphase Flow—Models for Nuclear, Fossil and Biomass Energy Conversion which I had been working on for the book series Advances in Transport Processes for the editor Professor Arun Mujumdar of McGill University and sent the manuscript to him. I had proposed this article to him when I was at LLL.

I joined ANL on March 2, 1981. Projects involving COMMIX-1 such as the thermal shock problem for nuclear pressurized water reactors (PWRs) had higher priority. After a while, I flat-out objected to working on single-phase flow and told Bill that the only reason I joined his group was to work on two-phase flow. He grudgingly relented, and then, I was allowed to work on COMMIX-2. The project was a mess. Although some progress was made, this code was never released and the conflicts with Bill were not conducive to a productive atmosphere. Almost all of Bill's group were Chinese and bowed to his every request. After he left EG&G Idaho, Inc., Wen Ho Lee had worked for Bill Sha, before I joined ANL, and he left before I joined after just one year. Maurizio Bottoni, a visiting scientist assigned to ANL from the German Nuclear Research Centre of Karlsruhe (KfK), with whom I worked on the COMMIX-2 code, has published his account of Bill Sha's behavior [26] which I highly recommend to the reader since it contains a good synopsis of my contributions to the code. Maurizio took it upon himself to document his version of COMMIX-2 [27]. A good 30–40% of this document was based on my notes. In summary, I can truly say that the time I worked in the Components Technology Division under Bill Sha was quite unpleasant. He would load me with impossible deadlines which caused me to work long days into the evening. He would round up his group on weekends to review progress and to prepare for upcoming meetings. To relieve my tensions, I would spend many hours talking with Hank Domanus, the true developer of all the COMMIX codes. Bill didn't abuse him, but he did dupe him by giving the impression to the outside world that he himself was the developer. Since Hank never went to any technical meetings he was unaware of this duplicity. In spite of the hardships which I bore while working under Bill Sha, I think I did make some significant contributions. I was principal investigator of two EPRI three-dimensional thermal and fluid mixing experiment analysis projects using the COMMIX-lA computer program, worked with Maurizio and Hank Domanus on modeling low pressure boiling modeling while developing the COMMIX-2 computer program, and helped to develop three-dimensional skew-upwind and volume-weighted skew-upwind numerical methods to reduce numerical diffusion in the COMMIX-1B computer program [27–31]. In 1981–1982, I proofed the galleys of my review article Multiphase Flow Models for Nuclear, Fossil and Biomass Energy Conversion (the editor removed the dash) which I received in late 1981. This was a rather time-consuming effort because of communication problems with the publisher which was in India. I did this on my own time, and it was published the next year [32]. In the fall semester 1982–1983, Darsh Wasan the Chair of the Chemical Engineering Department at IIT gave me an appointment as a part-time faculty member in the evening school. I developed and taught the course Multiphase Flow, ChE 552 which was broadcast on IIT/V. These notes were based on those I developed for a similar course I had taught in the night school of the Idaho Falls extension of the University of Idaho in Idaho Falls. There was one participant Laurel Briggs from ANL who took the course via television. Bozorg took scrupulous notes which I asked him to copy for me to supplement mine. I would use these notes to good use later as described below.

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Chapter 13
METC Starts Erosion R&D Cooperative Venture and MFIX Code Development Using FLUFIX Code

13.1 The METC Cooperative R&D Venture

Greg Berry in the Energy and Environmental Systems (EES) Division (later Energy Systems Division) met with me and described a project he was trying to initiate with Morgantown Energy Technology Center (METC), now National Energy Technology Laboratory (NETL). It would involve modeling erosion in fluidized beds. Even though I didn't know beans about erosion, I jumped at the opportunity to get away from Bill Sha. I explained to Greg my experience with modeling fluidized beds starting when I was at LLL and subsequently with Dimitri at IIT. He arranged for a meeting at METC on April 26, 1984, taking me and two others who were working with Greg on two other initiatives: Steve Choi on coal water mixtures and Professor Paul Chiu on group combustion modeling. Greg said that if I transferred to the EES Division and work for him on the erosion project, he would take care of all the paper works. Bill Sha went on vacation for several weeks in 1984. This was about the first time he had done so while I worked for him. Greg was able to accomplish this by pulling strings with the EES Division Director with whom he was on good terms. And so I transferred to the EES Division around July 1984 before Bill returned from vacation! Of course, Bill was furious to find I was gone, but Greg was able to keep him from reversing the fait accompli. I asked Bozorg to send me the version of the IIT code which he used for his Ph.D. thesis in anticipation that I might require it for the fluidized-bed erosion project. Dimitri and Bozorg developed a stabilizing solids pressure term not present in the initial version of the code. Bozorg then programmed it into the code in order to prevent the recurring overcompaction of solids below the packed-bed value of roughly 0.4 upon the fluidized-bed collapse. This overcompaction caused convergence and conservation of mass problems. In addition, this solids pressure term caused the one-dimensional equations to be become hyperbolic. Greg and I discussed what the name of the code should be. He offered FLUBED, but we decided a better name would be FLUFIX (no hyphens), to suggest its origin, and that is what we christened it.

R.W. Lyczkowski, *The History of Multiphase Science and Computational Fluid Dynamics*, Mechanical Engineering Series,
https://doi.org/10.1007/978-3-319-66502-3_13

I dug into the erosion literature assiduously and soon came to the conclusion it lacked a firm theoretical foundation. There were inconsistent correlations almost all a variant on the pioneering work of Ian Finnie [1, 2]. His model formed the basic pattern for all single-particle models. His major assumption is that a particle, approaching the eroding surface at some angle measured from the surface (called the impingement angle), would remove material in much the same way as a machine tool would. The particle is assumed to be much harder than the surface and doesn't break up. The surface material is assumed to deform plastically during the cutting process; hence, the material is defined to be ductile. And so I amassed all of the literature I could lay my hands on (this is before Google) to try to make sense of it. I tried to figure out how to apply these single-particle erosion models for erosion of the water-cooled tubes immersed in fluidized-bed combustors. One idea that appealed to me was the so-called power dissipation model used to analyze slurry jet pump erosion [3]. This model would lead to the energy dissipation model concept by discussions with Dimitri. The power and energy dissipation models are based on the very general consideration of erosion, resulting from energy transfer from the solids in a two-phase mixture to the eroding surfaces.

Michael (Mike) Petrick, who was, at that time, the program manager of the Fossil Energy (FE) in the Chemical and Materials Technology (CMT) Division at ANL, took it upon himself to build on the METC fluidized-bed erosion project in an initiative he was developing to address the problem of erosion which was occurring in fluidized-bed combustors. Fluidized-bed combustion (FBC), although it is an established means of burning high-sulfur coal and various other difficult-to-burn feed stocks in an efficient, cost-effective, and environmentally acceptable manner, had experienced erosion, i.e., wear or wastage, of in-bed components, such as tube bundles and water wall enclosures in many units. This wear is caused not by the coal particles but by the limestone which is introduced to take up the sulfur dioxide produced from burning high-sulfur coal. Several members of Mike's program Bill Swift and Erv Carls were currently assisting in a project involved with understanding the incredibly high tube failure rates in the IEA/Grimethorpe pressurized fluidized-bed facility in the UK [4]. This might have been the reason Greg was interested in the erosion project in competition with the CMT Division.

While I was busy enough working on the development of a fluidized-bed erosion model in conjunction with using the FLUFIX code, I was also called upon to help Petrick develop his proposal. Then METC sent a request to Petrick requesting technical assistance for their fluidized-bed computer code development. As described in Chap. 11, the DOE had spent several millions of dollars in an effort to develop such a code. METC personnel had been evaluating the S^3 CHEMFLUB code (they may have entirely dismissed the JAYCOR FLAG code), and they were not very happy with it. The principal investigator was Tom O'Obrien working with Professor Atul R. Padhye on assignment from WVU and who was in charge of the code evaluation. The documentation of the code by S^3 was incomplete [5] and that is why the BDM Corporation had been given the task of producing documentation from the source code [6]. The result was a disaster. Tom and Atul struggled for quite a while just trying to reproduce minimum fluidization which should have been a trivial task.

Part of the problem was that all they had were small VAX computers manufactured by Digital Equipment Corporation (DEC). The reason METC contacted the CMT Division at ANL was because it had a strong experimental fluidization program at the time. However, it did not have any modeling expertise. This request circulated around ANL and landed in Greg Berry's lap. He showed it to me, and I immediately told him and the EES Division Director that I was the only one at ANL who was capable of helping METC. I explained that I had been working on modeling fluidized beds starting at LLL and then at IIT. I applied for the opportunity by putting my qualifications in writing since I had to convince the CMT Division. There was a long-standing rivalry between the CMT and EES Divisions for funds and that caused some friction. After some time, they conceded that I would be the one to fill the METC request. No one else had applied as far as I know.

In early October 1984, I was put in touch with Tom O'Brien and Professor Atul Padhye to coordinate the logistics of the METC fluidized-bed assistance project and to define its components. Tom O'Brien initially wanted me to go to METC halftime for quite a long period of time. I told him I thought this was overkill. I put together a plan on how to transfer the FLUFIX code and get it running on their VAX computers from ANL without having to physically go to METC. Once that was accomplished, then I would deliver a five-day lecture series at METC for the week of November 12–16. After that I would visit METC as needed. Atul would be the person in charge of the computer work working with me. I sent Atul the plan I developed and an outline of the lecture series. Tom agreed on the plan, and the project got funded and started shortly thereafter.

I decided that it would be best if he and any colleagues who might get involved with this project to have accounts set up on the ANL computer system. In this way, we could transfer computer codes and data back and forth quickly and securely. This was before the advent of the Internet. The federal government had their own network-connecting government institutions. I sent Padhye the FLUFIX and K-FIX codes and input data sets. He sent me the CHEMFLUB code and input data for computing minimum fluidization. I set up protocols using the ANL WYLBUR and HISTORIAN systems for us to keep track of any changes that he or I might make to the codes, and to compile and run them. It took the better part of the month to shake down the procedures for compiling and running FLUFIX on the METC VAX computer. I hired Jacques Bouillard, a Ph.D. student of Dimitri's, to assist me. Bozorg was busy with postdoc activities with Dimitri and was not available. Jacques and Bozorg knew each other and had experience with the IIT code. We were able to compile the CHEMFLUB code on the ANL computer system. I explained to Tom and Atul that I had made a great deal of progress in transferring and running FLUFIX and that a shorter time would be appropriate for my stay at METC. We agreed that I would delay my lecture series at METC to December 10–14, 1984, and return at a future time if necessary. I went to METC on December 9, rented a car, and settled into a motel. The next day I drove to METC and started the lecture series. There were about a dozen METC participants. I was able to wrap up the lectures on Thursday, December 13 and return to Chicago. METC was now off and running with the FLUFIX code and double checking everything. For some reason unclear to me, Phil Nicoletti, a computer systems person at METC, and Atul performed a line-by-line comparison of the K-FIX and FLUFIX codes and eventually wrote a report [7].

After the visit to METC was over, I continued to assist Mike Petrick to develop his initiative. About May 1985, Mike rallied (demanded is his style) Walt Podolski and Carl Youngdahl in the FE Program, who were working on fluidized-bed and erosion experiments and instrumentation, and myself to go with him to METC on June 18, 1985, to make a pitch for his proposed initiative now titled Erosion in Fluidized-Bed Combustors. The components of the initiative included an erosion threshold study, a non-intrusive erosion monitor development, computer modeling (to be done by me) and fluidized-bed experiments. The deliverables promised were rather sweeping including computer software to optimize FBC designs for minimum erosion, guidelines for acceptable feed material characteristics and FBC operating conditions, and online devices to monitor erosion rates. These devices were to be ultrasonic thickness gauges to be placed inside selected water-cooled tubes extending the technology developed to monitor real-time erosion of tube bends externally.

Mike presented the introduction, Walt presented the overview of the project, and Art presented a description of the erosion threshold studies and monitor development. I made the presentation on computer modeling stressing that understanding solids motion was the key to predicting erosion. The FLUFIX code would be used as the basis to develop the hydrodynamic model. Some of the improvements would be to extend the two-dimensional code to three dimensions, to add solids and gas energy equations and multiple species, and to model flow around one and multiple tubes. The output of the FLUFIX model would feed into the FBC erosion model to be developed. The angle would be to build on the METC/ANL program on which I was already working. The FLUFIX computer code output would be used to produce erosion rates and FBC design guidelines. I threw in the kitchen sink on items that the code would be able to do even though I had no results to show at the time. Walt concluded the presentation by presenting the validation experiments that were to be performed in the IIT thin "two-dimensional" experiment and the computer-aided particle tracking facility (CAPTF) at the University of Illinois at Urbana-Champaign. It was a bravura performance by all and wildly oversold.

Essentially the same presentation was made to the Fossil Energy Industrial Advisory Committee at ANL on the morning of July 10. By that time Jacques and I had a *very preliminary* prediction of erosion rates around a rectangular obstacle placed in the IIT thin "two-dimensional" experiment. Common Wealth Edison showed interest in the erosion monitor device. The very next day Mike, Walt Podolski, Art Youngdahl, and I flew to Cleveland, Ohio, to talk about the proposal with Babcock and Wilcox (B&W) R&D in Barberton. On July 17, I sent a package of literature on my work modeling fluidization since 1979 to Dr. R.A. Mcllroy, with whom I had discussed the proposal. C.J. Baroch, Vice President, Advanced Energy Systems sent a letter to Mike on August 23, stating that a program such as was presented was needed but that some of the goals were somewhat over optimistic. B&W would be interested in participating in the program once a strategy with more participants was developed. Then on July 25 we all flew to New York La Guardia and drove to Stamford Connecticut to meet with Keeler Dorr-Oliver. After this meeting, we drove to Livingston, New Jersey, to meet on July 26 with Foster Wheeler Energy Corporation. Keeler Dorr-Oliver thought that the program was worthwhile, offered their endorsement but no financial support. Foster Wheeler thought the project was well thought out but that sufficient research was being conducted and was not interested in participating.

Getting money out of METC was like pulling teeth. So in the time after the blitz described above trying to sell the erosion project to FBC industry participants, Mike had us sharpen up the proposal. He set his sights on making another pitch to METC. On January 6, 1986, Petrick Walt, Art, and I went to METC to make a second presentation. Mike had contacted EPRI and Combustion Engineering. EPRI decided to start funding the erosion work to the tune of $50 k per year. This was the key to that started to convince METC that the project was worth funding. Now the project was centered around the hydrodynamic and erosion modeling. Combustion Engineering indicated a positive response in participating to do erosion testing. Jacques and I had made progress since the last METC presentation. The erosion literature was thoroughly scoured and consolidated, and we had developed a fluidized-bed energy dissipation erosion model. I came up with this MACRO/MICRO modeling procedure. The idea would have been to perform a MACRO hydrodynamic calculation treating the tubes as a distributed resistance concept. Then, MICRO calculations for hydrodynamics and erosion would be performed in critical zones in the fluidized bed driven by output from the MACRO calculations (see Appendix J, Figure 1).

It took Mike about another year to get all the pieces together. In 1986, a three-year Cooperative Research and Development Venture "Erosion of FBC Heat Transfer Tubes" funded with about a half million dollars from DOE METC came into existence. Every time I would meet with Tom O'Brien he would mutter "You got a half million out of us." The first steering committee meeting took place on May 27, 1987, at the Chicago O'Hare Hilton Hotel where the memorandum of understanding was signed. Members of the venture became DOE METC, EPRI, State of Illinois Center for Research on Sulfur in Coal (now the Illinois Clean Coal Institute), Foster Wheeler Development Corp., ASEA Babcock PFBC, ABB Combustion Engineering, Inc., Tennessee Valley Authority, British Coal Corporation, CISE, and ANL. IIT (Dimitri), the University of Illinois at Urbana-Champaign, and Babcock and Wilcox were also a part of the venture as contractors. Steering committee meetings took place quarterly.

During the period of time selling the Cooperative R&D Venture, I thought rather highly of Mike Petrick. He had expended all of this effort to showcase a lot of ideas I had proposed to him. Mike was replaced by Irv Carls as Fossil Energy Program Director and took over leadership of the Cooperative R&D Venture. Then Mike transferred to the EES Division to become supervisor over Greg Berry and me. His big project became the use of a large superconducting magnet that had been used in the magnetohydrodynamics (MHD) program for a crazy idea for MHD seawater propulsion for submarines. His attitude toward me became more and more hostile until I came to loath him. I can't pinpoint the exact reason he changed his attitude, but it may have been that I was becoming a threat to his supremacy, or else he took it out on me because of Erv's replacing him as Fossil Energy Director. Mike commandeered Jacques to work part-time on his seawater propulsion project.

An incredible amount of work was accomplished. However, a relatively small fraction of it was published. I hired four of Dimitri's Ph.D. students to assist me. Jacques Bouillard was the first whom I already mentioned. In addition, there was York Tsuo, Isaac Gamwo, and Jianmin Ding. I hired them, and they were working simultaneously on tasks I would assign to them. They all helped prepare the visuals for the quarterly steering committee meetings. After Jacques received his Ph.D. in 1985, I hired him as a postdoctoral appointee. Stephen Folga received his Ph.D. in 1986, the last one from the Gas Technology Department at IIT, and I also hired him as a postdoc. Tsuo, Ding, and Gamwo would receive their Ph.D.'s in 1989, 1990, and 1992, respectively. They would use portions of the work they performed in their doctoral theses. After he graduated, I hired Ding as a postdoc. ASEA Babcock PFBC funded Dimitri for a year to take data in the thin "two-dimensional" fluidized bed. After that they then decided to internally fund Babcock and Wilcox to develop a three-dimensional version of the FLUFIX code. The CAPTF experiments were funded by the State of Illinois Center for Research on Sulfur in Coal. Foster Wheeler Development Corporation modified one of their experimental facilities to measure pressure fluctuation and erosion rates in a shallow, variable thickness, fluidized bed. ABB Combustion Engineering performed the drop-tube erosion experiments since it was determined that ANL did not have the proper facilities. The erosion monitor device project failed because it was not possible to successfully weld the ultrasonic transducer to the inside of a tube which could withstand temperatures typical of a fluidized-bed combustor. ANL took on the overall management of the Cooperative R&D Venture. This effort produced the first multiphase erosion code EROSION/MOD1 [8]. It incorporated the monolayer energy dissipation (MED), Finnie, and Nielson-Gilchrist erosion models coupled with what would eventually become FLUFIX/MOD2 [9]. Thierry Karger, an exchange visitor at Argonne during the summer of 1985, assisted in producing the preliminary automated initialization procedures and generalization of the FLUFIX/MOD1 code (see reference 19 in FLUFIX/MOD2) [9]. Working closely with ANL, Babcock and Wilcox developed a three-dimensional fluid-solids computer code called FORCE2 which contained the FLUFIX equations and constitutive relations [10]. In order to accomplish most of the objectives, the Cooperative R&D Venture was extended to a fourth year.

I would use the notes I prepared for the lecture series at METC in 1984 as a basis for a FLUFIX/EROSION Workshop held at ANL on June 16–20, 1989. This Workshop was designated as one of the deliverables of the Cooperative R&D Venture. Invitations were sent out to representatives in September along with the outline developed for the Workshop for comments. There were three days of lectures on June 16–18 by Jacques Bouillard and myself. The lectures were interspersed with instructions on how the participants could have "hands-on" experience to set up and run sample problems accessing the computer FLUFIX and EROSION codes using procedures set up using the ANL WYLBUR and HISTORIAN systems. These codes are available from the Energy Science and Technology Software Center (ESTSC) at www.osti.gov/estsc. A separate ANL account was set up for each attendee. Two optional additional days were to follow the three days of lectures for those who wanted to stay to set up and evaluate additional problems and to engage in further discussions. A total of a dozen attended the Workshop which was acknowledged by METC as being well organized, pertinent, and generally well done.

The last steering Committee meeting took place on January 16, 1991, at the Chicago O'Hare Hilton Hotel. It would have been great if a national program could have resulted from this experience. The major deliverable of the Cooperative Venture was the erosion guidelines report. It went through many revisions, and the final report was assembled rather hastily and published by METC [11]. An opportunity arose for me to correct, to revise, and to update this report for Springer Briefs in Applied Science and Technology, Thermal Engineering and Applied Science to include many of the key publications resulting from the Cooperative R&D Venture [12]. I encourage interested readers to obtain this Brief because it forms an integral adjunct to this chapter. Related Funding from the Pittsburgh Energy Technology Center (PETC), now merged with NETL applied FLUFIX to the modeling of dense suspension (slurry) flows [13–15].

13.2 METC Starts the MFIX Code Development

Madhava Syamlal (known to all as Syam) received his Ph.D. from IIT in December 1985 under the guidance of Dimitri. I was on his thesis defense committee. He and Jacques Bouillard were classmates at IIT extending the work that Dimitri started with Bozorg Ettehadieh. They worked on Dimitri's grant from the DOE PETC. Jacques was one year behind Syamlal, receiving his Ph.D. in December 1986. Even before Syam formally received his doctorate, he was hired in July 1985 by Tom O'Brien and joined EG&G Washington Analytical Services Center, Inc. (later called EG&G Technical Services West Virginia, Inc.) in Morgantown. EG&G was what I call a captive contractor. He and Bill Rogers shared a trailer inside the fence next to METC Headquarters. There were also other trailers for other captive contractors. I would visit Syam and Bill on those occasions when I would travel to METC for review meetings for the Cooperative R&D Venture described above. Tom wanted to develop an in-house fluidization code. He already had FLUFIX. But by hiring Syam, he could build upon that code with the one that Syam developed for his Ph.D. thesis [16]. Syam extended the K-FIX solution algorithm to account for multiple particle phases and heat transfer to the walls of a fluidized bed. The original name for what was to become the MFIX code was NIMPF (<u>N</u>on-<u>I</u>sothermal <u>M</u>ulti<u>p</u>article <u>F</u>luidized bed) [17].

In 1998, Syam subsequently joined Fluent, Inc. as the Regional Consulting Manager for the captive Morgantown field office and simultaneously Research Group Leader, Multiphase Flows at NETL, the new name for METC, which for a while was called the Fossil Energy Technology Center (FETC). He is now Senior Fellow, Computational Engineering at NETL. He and Tom O'Brien have been instrumental in developing the open-source code MFIX (Multiphase Flow with Interphase eXchanges) starting in 1991. The main goal at that time was to develop a computer code to reliably model fluidized-bed reactors such as coal gasifiers, commonly encountered in fossil fuel plants. The major requirements of this code were the capability to do three-dimensional transient simulations and to produce a validated and documented code, as no commercial or open-source codes with such capabilities existed at that time. The first version inherited the numerical technique found in an early version of the IIT code [16, 18, 19] and was completed by January, 1993. Syam was responsible for a Cooperative R&D agreement between NETL and Fluent, Inc. for the transfer of multiphase technology into the FLUENT code which was executed in 1995. By 1997, the Fluent code with multiphase capability was released (see Chap. 14 for more about Fluent.) There continues to be a close relationship between NETL and Fluent, Inc. via the MFIX code development and technology transfer into the Fluent code. The public distribution of the code through the Energy Science and Technology Software Center (www.osti.gov/estsc) started in 1995. Later, Oak Ridge National Laboratory (ORNL) worked closely with NETL to parallelize the code. MFIX has bridged the transition from mainframe computers since the code runs in serial and in parallel on PCs, workstations, clusters, and what are now termed high-performance mainframes. A website, http://www.mfix.org, was launched in 2001 for distributing the source code and disseminating information related to computational gas–solids flow. NETL received an R&D 100 award for MFIX in 2007. The original version of MFIX was based on the two-fluid model and did not have a graphical user interface (GUI). Now, the code also includes the discrete element method (DEM), the particle-in-cell (PIC) method, and a hybrid method as well as a GUI. MFIX continues to be further developed and is available from the website https://mfix.netl.doe.gov. An up-to-date description of the MFIX capabilities and models is described in Chap. 2.7 in the Second Edition of the Multiphase Flow Handbook [20].

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Chapter 14
The Rise of the First Commercial CFD Codes: PHOENICS, FLUENT, FIDAP, CFX, FLOW-3D, and STAR-CD

14.1 PHOENICS Code

The CFD code development group at Imperial College headed by D.B. Spalding began multiphase flow modeling in the mid- and late 1970s [1]. Spalding developed the interphase slip algorithm (IPSA) to solve the PDEs contained in the PHOENICS code, debuting in 1978, which Runchal [1] claims "…was the first commercially available tool in CFD." Runchel makes extensive reference to the influence of the Group T-3 at LANL on multiphase flow, but does not mention the SLOOP code development work at ANC. This is in spite of the fact Spalding was quite aware of it as evidenced by his consulting at ANC in the early 1970s and his participation in Dimitri's 1976 NSF workshop [2] and the 1979 EPRI workshop [3] discussed in Chap. 8. The Web site for the PHOENICS code is http://www.cham.co.uk. Spaulding died just short of his 94th birthday on November 27, 2016 [4]. Hence, another giant in the area of CFD has left us, the first being Francis H. Harlow on July 1, 2016, whom I discussed in Chap. 5.

14.2 FLUENT, FIDAP, CFX, and FLOW-3D Codes

The FLUENT code started in 1983 by a small group at Creare, Inc., an engineering consulting firm in Etna, NH. The first commercial version was called CREARE X. It was developed by Prof. James Swithenbank and his team, including Ferit Boysan, at Sheffield University in the UK. The first version allowed for two- or three-dimensional structured grids using Cartesian or polar coordinates, steady-state flow, laminar or turbulent conditions, heat transfer, three-component combustion, a dispersed phase, natural convection, and an easy-to-use interactive front end. The first sale of FLUENT was made in December. In 1984, six more licenses were sold. Boysan launched Flow Simulations Ltd., in Sheffield UK, which later became

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Fluent Europe. In 1988, the Fluent group at Creare, Inc., formed a new company, Fluent, Inc., headquartered nearby in Lebanon, New Hampshire. In 1995, Fluent, Inc., was acquired by Aavid Thermal Technologies and became a wholly owned subsidiary. In May 1996, Fluent, Inc., acquired Fluid Dynamics International located in Evanston, Illinois, which developed the FIDAP finite-element code and in 1997 acquired Polyflow S.A., developer of the POLYFLOW code. As mentioned in Chap. 13, Madhava Syamlal was instrumental in the transfer of multiphase technology developed in the MFIX code into Fluent in 1997. It includes Dimitri's granular flow model [5], unstructured mesh capabilities for transient and steady state, and serial and parallel computations.

The CFX code, formerly named FLOW-3D, was developed at the United Kingdom Atomic Energy Authority at Harwell and in 1996 was privatized in the US at AEA Technology Software Engineering, Inc. The reason for the name change was that Tony Hirt, who founded Flow Science, Inc., in 1980 when he left LASL, had previously trademarked their FLOW-3D code in several countries. He convinced AEA Technology Software Engineering, Inc., to change the name to CFX. Their documentation clearly showed that they had prior use of the name. Tony sold Flow Science, Inc., in 2000 and now devotes his time to developing novel applications for FLOW-3D. Their Web site is at www.flow3d.com. ANSYS, Inc., acquired CFX in 2003, and it is now called ANSYS® CFX®. AEA Technology Software Ltd., located in Waterloo Ontario Canada appears to continue licensing its own version of CFX. Fluent become the largest supplier of commercial CFD software in the world and in May 2006 was also acquired by ANSYS, Inc. The development of Fluent has continued to the present version now called ANSYS® FLUENT® 18.0 having moving geometry, large eddy simulation (LES) turbulence modeling, and solution optimization. For a full list of ANSYS capabilities, the reader is encouraged to visit the ANSYS Web site at www.ansys.com.

14.3 STAR-CD

In the middle of 1980s, David Gosman together with Dr. Raad Issa formed Computational Dynamics Ltd., with the aim of developing an unstructured body-fitted industrial CFD code. Adapco, a New York-based structural engineering consultancy company, backed Computational Dynamics to produce a commercial body-fitted CFD code named STAR-CD® (which stands for Simulating Transport in Arbitrary Regions). The first version was block-structured but, by its second release in 1991, STAR-CD had been recreated to become the first truly unstructured commercial code, offering engineers the ability to construct meshes from any combination of hexahedral, tetrahedral, and prismatic cells and thereby providing geometrical and meshing flexibility. STAR-CD quickly became the default CFD code for the simulation of engine combustion problems.

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Part IV
Attempts to Establish a National Program for Multiphase Flow Research

Wherein is told of several failed attempts and a faltering success.

Chapter 15
The Failure of Argonne National Laboratory to Establish the Multiphase Flow Research Institute

In 1984, Bill Sha in the CT Division at ANL started an initiative to be called the Multiphase Flow Research Institute (MFRI). This initiative started at about the same time that Mike Petrick in the CMT Division at ANL was starting his initiative to address the erosion issue in fluidized-bed combustors. The history of Petrick's initiative culminating in the Cooperative R&D Venture is thoroughly discussed in Sect. 13.1. This is a perfect example of one ANL division pitting itself against another division in an attempt to garner funds from the government. Unfortunately, such a self-aggrandizing rivalry is harmful because cross-messages go out to the DOE from such a rivalry. Of course, the stronger man wins. Bill was not the stronger man. What follows is the recounting of Bill's failed attempt.

To be sure, Bill's aims were higher on paper than Mike's. This is similar to his code development philosophy for the COMMIX-2 code which was to build upon a strong foundation without true substance or understanding. On May 15, 1984, while I was still in Bill's Analytical Thermal Hydraulics Research Program (ATHRP) group, he circulated a draft of a document titled Preliminary Proposal for the Formation of Multiphase Research Institute at Argonne National Laboratory. The Multiphase Research Institute (MRI) was the original name for the MFRI. In the draft proposal for the MRI, Bill had as its mission to "Enhance the knowledge of 'Multiphase Thermal Hydraulics' which is generally applicable to energy-related fields, e.g., nuclear reactors, fusion systems, fossil energy, solar energy, etc.". He set himself up as the Chair of the Board of Directors with the late Professor James P. Hartnett at the University of Illinois Chicago as Cochair. Vipin Shah a member of Bill' ATHRP group was to be Executive Secretary. He identified six ANL personnel (none from the EES Division) and six distinguished university professors who would serve as members of the Board for an initial period of three years. I should note that the six professors named were mostly consultants for Bill's code development group, all from nearby Midwest universities. And where would the income come from? Why of course, the DOE Office of Basic Energy Sciences (BES), the NSF, etc. Bill was envisioning an income level around $4 million per year in the "growth phase" of the MRI. Research proposals would be invited from

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universities and ANL. As the reader can surmise, Bill had made no small plans and intended that he would be the boss. On August 1–3, 1984, he visited the DOE BES and the NRC. Dr. Oscar Manley who was at that time in Director of DOE BES Multiphase and Particulate Research encouraged Bill to submit a proposal and to include Mamoru Ishii at ANL whom Oscar was already funding. On August 24, Bill issued a memo to which he attached the minutes of his meeting of the August 17, 1984, he convened with the six ANL personnel identified in his May 15 document to inform them of his trips to DOE BES and NRC and to define the components of his large laboratory-wide proposal on multiphase. Then shortly after he and Vipin Shah sent memos to a large number of ANL personnel requesting 2- to 3-page proposals on research topics of their choice in the areas of multiphase flow and heat transfer.

In June 1985, Jim Hartnett, Secretary of Midwest Universities Energy Consortium, Inc. (MUEC), sent a letter to members of the Research Committee enclosing the minutes of a June 5 meeting held at ANL. Professor Richard Goldstein, Chair of MEUC, refers to a March 1985 meeting of the committee (which I don't have) stating that much progress had been made since then. A review of technical summaries received organized them into two broad areas: fluid–fluid and fluid–solid systems together with priorities within each area. Hartnett was asked to prepare a carefully worded RFP which would be mailed throughout the Midwest region.

On August 16, 1985, a flyer titled Request for Proposal Abstracts (RFPA) Collaborative Research in Multiphase Flow Systems Phenomenological Modeling and Interfacial Phenomena was circulated throughout ANL. This flyer was issued by the Midwest Universities Energy Consortium, Inc. (MUEC) and ANL. Bill was listed as Cochairman. The avowed objective was to submit a major proposal to one or more federal agencies for the purpose of establishing the MRI in the Midwest and to announce the solicitation of two-page proposal abstracts to be sent to Jim Hartnett or Bill by October 1, 1985. Universities eligible to participate were members of MUEC in the states of Illinois, Indiana, Iowa, Michigan, Minnesota, Ohio, and Wisconsin. It was clear that it was the responsibility of ANL personnel to "beat the university bushes" for collaborators. However, universities could submit their own proposals with ANL collaborators.

On September 30, 1985, Dimitri submitted an abstract to Jim Hartnett titled Prediction of Nukiyama's Pool Boiling Curve in collaboration with me. He must have gotten the RFPA in the mail or from me. He felt that if Syamlal could predict wall to fluidized-bed heat transfer coefficients, sometimes termed a boiling bed, then it should be possible to predict the classical Nukiyama boiling curve [1]. On the same day, Walt Podolski, with whom I was worked with to establish the Cooperative R&D Venture with Mike Petrick described in Sect. 13.1, submitted a proposal to Bill Sha titled Investigation of Gas-Solids Flow in Fluidized Beds with me as second author followed by S. Saxena from the University of Illinois Chicago, and Mike Chen and B. T. Chao from the University of Illinois Urbana–Champaign. Most of the wording was taken from presentations made to try to sell the Cooperative R&D Venture.

On February 12, 1986, Hartnett sent a letter to the abstract review committee attaching the minutes of the January 30–31 meeting which reviewed the 56 abstracts which were received. Dr. Ken Kliewer, Deputy Director of ANL, opened the first day of the meeting. He stressed the importance of the industrial component in the development of the proposed research program. The only industrial representative on the abstract review committee was a person from General Motors who chaired this committee. The proposals were subdivided into two groups: 1. liquid–vapor systems and 2. fluid–solid systems. Then, they were ranked on how they achieved the three areas critical to the program: (1) phenomenological modeling, (2) measurement and experimental techniques, and (3) mathematical modeling and computational techniques. Sixteen proposal abstracts were accepted. Two of them involved Bill Sha, and three more of them involved members of Bill's group for a total of five out of the sixteen for just over 30%. Although several of the proposal abstracts involved collaboration with industry and other research institutions including national laboratories, none of them were among the sixteen that were successful. In my opinion, this was a fatal flaw. Even the one proposal that had a General Motors collaborator was rejected. I'm sure the unsuccessful applicants must have sensed that the multiphase initiative was skewed toward Bill Sha's group.

On February 14, 1986, our proposal abstract was accepted by Hartnett and Sha but had to be more focused and therefore needed to be revised. It was emphasized that the major objectives for the proposed multiphase flow program were: (1) improve predictive capability in designing multiphase flow systems and (2) an improved understanding of scaling multiphase flow systems. Dimitri's proposal was rejected by Hartnett and Sha on February 20. On March 4, Walt Podolski sent the revised version of our proposal to Bill Sha. On April 8–9, a meeting was held to review the revised proposal abstracts. On June 23, Hartnett sent a letter to members of our proposal with Podolski telling us that the initial budget request for the eight proposals selected for the solid–fluid category was to be $2.5 million for the first and second years of the proposed program. In case this full amount was not received, two budgets should be submitted: one for an optimum effort and one for a minimum effort. They were to be submitted to him by July 15, 1986. On September 23, Harnett sent a letter to Paul Raptis and L. S. Fan leaders, of the solid–fluid group, transmitting to them correspondence from the DOE concerning the proposal presentation made in August. Hartnett requested information concerning research ongoing that was funded by them. Here was another fatal flaw. Sha and Hartnett were unaware of what the DOE was interested in and what they were already funding. The proposals would only serve to disrupt an already well-oiled system of investigators familiar to the DOE. The ANL-MUEC proposals would only serve to muddy the waters. The letters received from DOE Fossil Energy and PETC were worded nicely but what they were implying, therefore, was that they were not really interested in the initiative.

An ANL proposal dated November 1986 titled ANL-MUEC Multiphase Flow Research Institute Solid-Fluid Multiphase Systems Research Component Volume I was submitted to Marvin Singer at the DOE. It contained a collection of the eight solid–fluid proposals. The one with Podolski, me, and Saxena, Chen and Chao from the University of Illinois Chicago and Urbana–Champaign was included. It was apparent that a lot of work went into this proposal. Prefacing the eight proposals containing resumes of the principal investigators was an introduction covering the background of the initiative. A time table of events indicated that the liquid–vapor/liquid–gas proposal was submitted to DOE BES in September 1986. The requested budget was for a total of $6 million per year: $3 million per year from DOE Fossil Energy for the solid–fluid multiphase systems research component and $3 million per year from DOE BES for the liquid–vapor or liquid–gas multiphase systems research component. I don't think much of anything happened because on March 25, 1987, Podolski submitted a revision of our proposal to Raptis which was now titled Dynamics of Turbulent, Dense Solid-Gas Flows. It now contained a list of milestones for a three-year proposal. On April 12, Podolski sent me another revision of our proposal which included changes requested by Raptis and Fan. The pagination (pages 56–77) indicated that it was now a part of a larger document, perhaps a revision of the November 1986 proposal. On July 27, 1987, Podolski submitted yet another revision of our proposal to Raptis. This is where the paper trail ended at least for the proposal. It was never funded. The Cooperative R&D Venture described in Sect. 13.1 had already started.

But hold on, the MFRI still lives! In 1987, the flyer for Cycle II Request for Proposal Abstracts for Collaborative Research in Solid/Liquid/Gas Multiphase Flow Systems was issued by the MFRI which the flyer stated was established in 1987. The proposals once again were to be sent to either Hartnett or Sha by October 15, 1987. It looked like the whole thing was starting all over. Like a fool, I involved myself with no less than three collaborative proposal abstracts. The most fully developed was titled The Use of Carbon Dioxide in Coal Slurry Transportation, Comminution, and Beneficiation submitted by Purdue University. The second was submitted by Chi Wang titled Investigation of Thermal Hydrodynamics and Wear in Solid-Liquid Systems. It involved Dimitri. I submitted Multifunctional Multiphase Fluid/Solids Analysis Program also involving Dimitri. I was informed by Sha on May 5, 1988, on MFRI letterhead that my proposal was rejected.

In 1989, Bill Sha presented a paper purporting to review the status of the collaborative research program in the multiphase flow area between MUEC and ANL [2]. He summarized six projects in the solid transport area he says started in FY 1989, i.e., October 1, 1988. There is no mention of the liquid–vapor/liquid–gas proposals. The source of funding is not mentioned, but he acknowledged Shelby Rogers, program manager from PETC "…for his support." This "support" could be interpreted a couple of ways, one of which is encouragement and the other is financial. Four of these six proposals were contained in the November 1986 proposal mentioned above. In Introduction, Sha stated "One of the missions of the MFRI is to streamline the research activities, with particular emphasis on *cohesiveness*." Whether these six projects are actually part of the collaboration is not entirely clear. They may have received funding independently and that He was trying to convince the NSF and/or DOE that he still had a program but in fact it was just a shadow organization. In 1990 Sha and authors of two of the projects which

"…made significant progress…" presented a paper [3]. These projects were led by R. J. Adrian and L. S. Fan. In fact, Sha's contribution to this paper was only in writing the abstract, The rest of the paper comprised two separate papers by each of these projects. By rights Sha's name should have been last. Recently I contacted L. S. Fan to ask him if he had a recollection of what happened with the MFRI. He was one of the leaders of the solid/fluid group. He told me that he was indeed funded by a grant from the DOE through the MFRI for the project Bubble-Wake in Gas-Liquid-Solid Flow. This was the same situation with Adrian who published a summary of his work accomplished by his grant [4]. There was nothing reported at the 1991 NSF-DOE Workshop. What happened to all of the other projects is not known to me. In December 1992 Bill was relieved of his administrative responsibilities and Richard Valentin was appointed Acting Section Manager of the ATHRP. This concludes my story of Bill Sha's MFRI.

After this fiasco, I became involved for a couple of years with a project modeling two-phase slurry flow. This was a very interesting and novel extension of gas–solids modeling for me. The trick was how to modify the rheology of the solids phase to account for the non-Newtonian behavior exhibited by liquid–solid slurries. The approach taken was a phenomenological one using empirical fits for the apparent viscosity as a function of shear rate. Because the carrier fluid was Newtonian, its viscosity could be taken to be a constant under isothermal conditions. The non-Newtonian shear rate dependence for the slurry was ascribed to the solids-phase viscosity. The first published paper analyzed coal water slurry data using a modification of ANL's FLUFIX computer program [5]. Then, the research broadened to analyze fundamental slurry data taken by magnetic resonance imaging (MRI) [6, 7]. Jianmin Ding, who worked with me on the Cooperative R&D Venture described in Sect. 13.1, transferred to Sha's group after its conclusion. It was he who programmed the two-phase slurry model and performed the calculations using a version of the COMMIX-M code with my guidance. Both of these projects were funded by the Pittsburgh Energy Technology Center (PETC) later to be renamed NETL (as was METC). The approach used in these three papers to model dense slurry flow would later serve as the basis for modeling blood flow called hemodynamics [8–10]. This subject will be discussed further in Chap. 20.

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Chapter 16
DOE OIT Virtual Center for Multiphase Dynamics Effort Begins—Becomes the Multiphase Fluid Dynamics Research Consortium

The Virtual Center for Multiphase Dynamics (VCMD) effort was a near miss on the national level and the Multiphase Dynamics Research Consortium (MFDRC) was a qualified success on a regional level. That is why I am going to trace their histories in some detail as I was intimately involved with their development. This chapter demonstrates some of the pettiness displayed by honest scientists, engineers, and technical leaders. This is part of the continuing saga of the politics of science.

In 1994, the American Chemical Society began participating in an effort to develop a vision document identifying the technology needs of the US chemical industry [1]. The document was to contain a road map delineating the mechanisms whereby those needs could be met. The idea put forward was to brainstorm the chemical industry's common needs and goals and thereby have the opportunity of individual chemical companies to view each others as partners rather than competitors. Certain broad-based technology needs could be met through forming consortia of companies to share resources.

To some extent, this kind of activity had already been going on since 1993 with the formation of the Chemical Process CFD (CPCFD) Users Group but on a much smaller scale. The CPCFD was under the sponsorship of Cray Research, Inc. (CRI) headquartered in Eagan, Minnesota. Richard LaRoche was the person responsible for assembling and running the meetings which were held twice a year in the spring and in the fall before the snow flies. Besides CRI, this group was comprised of four major chemical companies: Dow Chemical, Dow Corning, Eastman Chemical, and Dupont; a pharmaceutical company, Eli Lilly; a broad-based manufacturing company, FMC; a mixing tank company, Chemineer; a petrochemical/petroleum company, Shell Development; and National Institute of Science and Technology (NIST). Dow Chemical suggested the idea of forming this group to CRI in 1993. The group was very informal with no monies exchanged. The hosting company rotated, and all member institutions participated at their own expense. All information that was presented and exchanged was considered to be non-confidential and had to be cleared by the individual companies. CRI supplied some free computer time to members. The CPCFD Users Group activities were

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devoted exclusively to modeling laminar and turbulent nonreactive mixing tanks using the features of mainly three commercial CFD codes (FLUENT, FLOW3D (later called CFX), and FIDAP) and feeding comments and suggestions back to the vendors who are explicitly excluded from attending the meetings.

In 1995 Herschel Reese from Dow Corning contacted me to see if I was interested in participating in the CPCFD Users Group. I was invited to attend and make a presentation at the 5th Chemical Process CFD (CPCFD) Users Group Meeting hosted by CRI to be held at their Corporate Research Headquarters, May 23–25, 1995. In order to attend, and presumably to join, I had to submit an outline on what might ANL's role would be and what I proposed to talk about. Agreement from the CPCFD members had to be unanimous. I put together the following outline for discussion; 1. Define state of the art in multiphase fluid–solids modeling. 2. Define experimental needs and instrumentation, e.g., NMR, capacitance probes, X-rays, gamma-rays. 3. Experimental data acquisition and management. 4. Experts on interpretation of multiphase phenomena. 5. Define additional CFD code development and model validation needs and perform small-scale experiments using experimental facilities and techniques unique to ANL. 6. Define additional multiphase research needs with respect to multiphase theory, e.g., "turbulence," deterministic chaos, and scale-up. 7. Cadre of multiphase experts to draw upon as consultants. 8. Education as to solutions possible through workshops, short courses, and hands on computer laboratory. 9. Advisors to commercial CFD companies needs. 10. Bridge communications breakdown between operating plant staff, industrial R&D groups, and academia. The title of my presentation was CFD Modeling Capabilities at Argonne National Laboratory for Reacting Fluid–Solids Systems. The outline I developed above was not explicitly discussed at the meeting. The CPCFD had a charter which is contained in Appendix H. I would continue to attend these CPCFD Users Group meeting for the next several years when Cray Research became a wholly owned subsidiary of Silicon Graphics, Inc. to involve it in future activities in the formation of a Virtual Center for Multiphase Dynamics to be discussed in Sect. 16.2.

Starting in 1995 there was a serious effort supported by the DOE Office of Industrial Technologies (OIT) to establish what would eventually be called the Virtual Center for Multiphase Dynamics. There was a growing perception at the national level that CFD computational technology, including multiphase flow, was critical to meeting the future challenges of the US chemical industry. The first step in this process was a workshop held in the Computational Testbed for Industry at LANL on May 18–19, 1995 titled Reactive Multiphase Flow Simulations [2]. Approximately 35–40 people invited by LANL attended this workshop including 21 participants from 12 companies representing the petroleum, chemical, environmental and consumer products industries, two representatives from the DOE Office of Industrial Technologies (OIT) including Brian Volintine (who later changed his name to Valentine) and several from LANL. Most of the presentations were made by LANL personnel to showcase the laboratory's capabilities. The avowed purpose of the workshop was to start a dialog between LANL and industry to try to find common needs and complimentary capabilities that could form the basis for the initiation of a coordinated effort to substantially increase the state of the art of multiphase CFD. Such an effort should benefit both private industry and the US defense complex which, by the way, LANL plays a critical role in nuclear weapons development research. If successful, such an effort would involve not only LANL and private industrial partners but also other government laboratories and partners from academia. Ed Joyce from LANL reviewed the 1st Industrial Energy Efficiency Symposium and Expo held May 1–3, 1995 in Washington, DC. It was at this meeting that the DOE-OIT unveiled their Industries of the Future Program which included chemicals, petroleum refining, forest products, glass, aluminum, metal casting, and steel, all recognized as heavy consumers of energy. It was also at this meeting that the seeds were planted for "virtual laboratories" constituting collaborations between industry and national laboratories for the Industries of the Future Program. Tyler Thompson from Dow Chemical, Cooperative Research, who would play a leading role in the formation of the future Multiphase Dynamics Research Consortium (MFDRC) to be discussed later, gave a presentation on some of his thoughts for a potential CFD consortium. Included in Appendix 11 containing Tyler's thoughts was a report, a sort of white paper, dated June 27, 1995 authored by Tyler and another colleague from Dow Chemical, Joseph D. Smith, titled Computational Dynamics for the Chemical Processing Industry. This white paper outlined the problems with existing computational packages as well as some of the challenges for the chemical process industry in modeling specific chemical systems. At the close of the meeting, it was decided that the next step would be to issue a white paper on the formation of a consortium based on the ideas put forward at the workshop. The white paper would be used to explain the mission and structure of a consortium and to lobby the government for funding.

No other national laboratories were invited at this meeting. As I remember this initiated a firestorm of criticism at ANL and presumably from the other national laboratories that LANL could be so blatant as to unilaterally initiate such an effort without inviting them to participate in the dialog on government–industry collaboration. The intention might have been there via Tyler Thompson's efforts, but the execution on the part of LANL was not in good taste.

16.1 Computational Fluid Dynamics Technology Roadmap Published as Part of VISION 2020

The next step in the Virtual Center for Multiphase Dynamics story concerns the chemical industry's initiative on getting involved in the DOE-OIT Industries of the Future Program. A report was assembled emanating from a meeting held May 23–24, 1995 in Washington DC by the chemical industries Technology and Manufacturing Competitiveness Task Group (TMCTG) [3]. The sponsors were the American Chemical Society (ACS), Chemical Manufacturers Association (CMA), American Institute of Chemical Engineers (AIChE), and Synthetic Organic

Chemicals Manufacturing Association (SOCMA). The objectives of the meeting were to achieve a critique of their draft vision and roadmap materials and to improve their Vision 2020. The TMCTG, under the chairmanship of John D. Oleson from Dow Corning Corporation, had been working since 1994 on Vision 2020 and a roadmap of change for the chemical industry. He was an outspoken leader in the chemical industry and shortly before this May 1995 meeting, testified before a House of Representatives Committee to explain his reasons why there should be partnering between industry and government [4]. He gave examples of Dow Corning's cooperative research projects with the national laboratories.

This Vision 2020 was intended to promote cooperation among industry members, their customers, and suppliers, and between industry and government. There was a short section titled Computational Fluid Dynamics (CFD) apparently authored by Steve Weiner from Pacific Northwest Laboratory (PNL). It also appeared as part of Appendix 11 of the Reactive Multiphase Flow Simulations document [2]. The main thrust of the vision statement was to guide and shorten the cycle for experimental optimization and scale-up for the chemical process industry (CPI). The report assembled from the May 1995 meeting was published in 1996 thus becoming the "roadmap: for the CPI [5]. The Council for Chemical Research was added as one of the corporate authors. The section on Computational Technologies is quite explicit as to the role that CFD would play in complex systems such as high-temperature gas-phase systems, multiphase mixing, polymer processing, non-Newtonian rheology, dense multiphase turbulent flow (with or without chemical reaction), and crystallization with particle nucleation and growth. This is due to the fact that results of the workshop "Reactive Multiphase Flow Simulations" [2] as well as the Thompson/Smith white paper contained in Appendix 11 titled Computational Dynamics for the Chemical Processing Industry provided input for the discussion of computational technologies. Following this May 1995 meeting there a Laboratory Coordinating Council meeting on June 21, 1995 in Washington DC where Steve Weiner made a presentation titled "Chemical Industry Visioning." He reviewed the above TMCTG efforts and milestones concluding with the release of the final version of Vision 2020.

16.2 The Attempt to Establish a Virtual Technology Multiphase Laboratory

I became involved with the Virtual Technology Multiphase Laboratory process due entirely to Brian Volintine at the DOE OIT. I knew him from my activities in the AIChE Heat Transfer and Energy Conversion (HT&EC) Division in the starting in the 1980s. I would work with him to prepare the Division Newsletter, to coordinate programming activities sponsored by the Multiphase Flow (Area 7 g), and to assist him in editing the AIChE Symposium series volumes for AIChE papers presented at the 27th through 29th National Heat Transfer Conferences held in Minneapolis, San Diego, and Atlanta in 1991 through 1993. So it was in September 1995 that I was personally requested by Brian to review the LANL white paper [6] which preparation was promised at the conclusion of the Reactive Multiphase Flow Simulations workshop discussed above [2]. One area where the government had been a clear leader through its national laboratories was in the area of multiphase dynamics. This white paper promulgated the formation of a virtual laboratory concept to advance multiphase dynamics. The intent of this concept was to maximize the DOE's return on its investment, and to serve as a model for moving other technologies from basic research to the applied arena. It was suggested that such a Virtual National Laboratory would embody a partnership among US government agencies, including the national laboratories, private industries, professional societies, and universities, which have needs for solving complex problems in multiphase fluid flow.

16.2.1 First VTC "Kickoff" Meeting November 28, 1995

The first meeting devoted to developing this Virtual Technology Center for Multiphase Dynamics (the name and/or acronym would change until the definitive one was decided upon) was held November 28, 1995 in Washington DC. I attended the meeting accompanied by Richard Valentin, director of the Components Technology Division as ANL representatives. It was held in a rented office at 655 15th St., NW a short distance from the White House. Whoever arranged for the venue forgot to order a viewgraph machine, and in spite of promises that it would show up, it never did. The room was too small, barely accommodating the 19 representatives from just about all the major laboratories. The attendees were (beside LANL and ANL), BNL: Upendra Rohatgi, INEL: Rod W. Douglass, LBL: Karsten Pruess, METC: Tom O'Brien, ORNL: W. Harvey Gray and Cloyd Beasley, PETC: Walter Fuchs, PNL: James A. Fort and Steven C. Weiner, SNL: Art Ratzel and Nancy Jackson.

Many participants showed up late because of poor directions (part of the building was being totally rehabbed and was ripped up). The meeting was steered by Ed Joyce from LANL who welcomed all. Accompanying him were Bryan Kashiwa, Brian VanderHeyden, and Dan Butler. Brian Volintine from OIT was late so the meeting started with Bryan Kashiwa, billed as the author of the plan described in the White Paper [6], who reviewed it. He used the word code initially, (later switching to the phrase CFD code library) to be the product and that it would be a living thing. He gave examples of similar prior and existing national laboratory industrial partnerships. The preferred name for the initiative at the time seemed to be "Center" rather than Virtual National Laboratory.

Brian Volintine gave a short overview of the DOE OIT, which organization was unfamiliar to many participants. He explained that the Reactive Multiphase Flow Simulations workshop [2] held in May at LANL could be viewed as a scoping investigation to find if there was interest in the present initiative. The conclusion was that there was a very strong interest. He explicitly mentioned that Ed Joyce would be developing the plan, and that I would be assisting him. Any feedback, comments, and concerns should be forwarded to Ed Joyce. Steve Weiner made some pithy comments. He said that the payback on industrial buy-in is in the applications. Several groups of national laboratories would bring together their capabilities synergistically. They should not start a new. To encourage industrial investment, products and utility must be coming out in the short term. The initiative should have a finite life, e.g., 10–15 years. Most work would be in subcode development. The visioning documents should be looked at for a match of multiphase objectives and industry needs, e.g., the chemical process industry, also the high performance center for computing.

Next ten laboratory representatives gave 15–20-min reviews of capabilities, examples of interlaboratory cooperation, and rough estimates of full-time equivalent (FTE) personnel working in multiphase. These FTE numbers ranged from four (METC) to 25–30 at ANL. One laboratory not on the tentative roster, LBL was represented, and one did not show up, Rose C. McCallen from LLNL, because she could not make it and thought the initiative was a good idea. Rich Valintin reviewed the "Dallas Team" purpose and findings developed over the last three years. The "Dallas Team" is a group of representatives from the national laboratories that facilitate the development of Virtual Technology Centers (VTCs), previously called Technology Core Competency Centers or TCCC). A VTC is a collection of core competency resources within a set of national laboratories that enables the conduct of focused R&D. Rich Valentin also made a presentation which I helped him prepare outlining ANL's CFD capabilities and status. The two biggest problems envisioned by the participants for a Virtual Technology Laboratory were intellectual property rights and ownership for the major product, the CFD code library. Several energy research (ER) laboratories, i.e., nondefense, including ANL LBL, and BNL, expressed fear that if ERs are not involved, there would be great problems getting the center started. Finally the discussion centered on where to go next. It was decided to develop a definition of multiphase capabilities for the national laboratories and match them with industry needs, most clearly defined, thus far, in the Industries of the Future visioning documents, e.g., petroleum, chemicals, forest products, steel. A clear statement of goals and a draft Memorandum of Cooperation should be drafted and presented at the next Laboratory Coordinating Council Meeting which was to be held December 6 and the next meeting of the "Dallas Team" on December 13.

16.2.2 Laboratory Coordinating Council Meeting December 6, 1995

Ed Joyce made the presentation Update on Virtual Laboratory for Multiphase Dynamics at the Laboratory Coordinating Council held in Washington, DC on December 6, 1995. He reviewed the November 28th meeting discussed above.

He summarized the observations of the meeting as: (1) The effort to establish a Virtual Laboratory would require the laboratories to integrate and assess capabilities, both internally and externally. (2) The laboratories have strong capabilities in both theory and experiment, with a broad applications basis. (3) Many participants felt that the proper approach to a product would be a library of computer codes. The major action items decided upon were to develop mission and vision statements; a list of laboratory's capabilities, programs and accomplishments; and a memorandum of cooperation. The draft Mission Statement that he presented was as follows.

"DRAFT" MISSION STATEMENT

The VTC for Multiphase Dynamics integrates and develops the resources of Industry, Government, Academia and Professional Societies, to enable reliable analysis in multiphase dynamics. Application areas include process design, process control, with implications to conservation of resources, and minimization of environmental impact. This will be accomplished by a focused effort to obtain a fundamental understanding, and the use of this understanding for solving problems crucial to industrial competitiveness, environmental remediation, and national security

The "Draft" capabilities list presented was as follows:

"DRAFT" CAPABILITIES LIST

By the year 2006 the VTC will have brought Multiphase Dynamics into the realm of an enabling technology. As such, the VTC membership will have the capability to predict with confidence the performance of unit operations to be used in processes for creating chemicals and materials. The performance prediction will be comprehensive in that it impacts on the environment and on resources will be discernible.

The primary means by which the VTC focus will be maintained is by the creation, support, and validation of a computer simulation capability for multidimensional, time-dependent problems in complex multiphase flows that arise in problems important to the VTC membership.

The "Draft" capabilities list presented was as follows:

"DRAFT" CAPABILITIES LIST

- Numerical methods for multiphase flow.
- Closure and constitutive theory and modeling - turbulence and exchange.
- Experimental methods for multiphase flows - advanced diagnostics.
- Multiphase flow applications - industry, environment, national security.
- Parallel computation methods for multiphase flows.

16.2.3 Second VTC Meeting December 13, 1995

The next meeting held was the Virtual Technology Center for the Investigation of Multiphase Dynamics "Dallas Team" Meeting held in Dallas, Texas on December 12–13, 1995. I attended this meeting as the representative from ANL and collaborator with Ed Joyce at LANL for the VTC initiative. The review of what was billed as the computational fluid dynamics working group was presented by Ed Joyce on the second day of the Virtual Technology Council or so-called Dallas Team meeting. The meeting on December 12 was not open to the Multiphase VTC. Dean Waters chaired both meetings. The “Dallas Team’s” function was to serve as advocates for the VTC concept, be the focal point for identifying starting VTC’s, maintain consistent generic VTC documentation models, and interface with the DOE.

The session to discuss the next steps to support the computational fluid dynamics working group effort followed Ed Joyce’s presentation. Dean Waters stated that there should be two chairs from two laboratories to form the center. This would ensure that if one chair does not carry through on action items and important milestones and the initiative gets bogged down for some reason, the other could take over. Having two chairs also illustrated cooperation. Ed Joyce, Dan Butler, and myself then left the meeting room. At lunchtime, Ed said that he was asked gently but definitively to leave the meeting until the afternoon session reserved for a facilitated meeting with the CFD working group. The other laboratory representatives arrived during the lunchtime, and then, we met informally in the hotel lobby restaurant. Ed Joyce said that the Dallas Team was somewhat shocked that so much progress was made so quickly without their guidance.

At the afternoon session, the representatives from the laboratories introduced themselves. The representation from the eleven national laboratories was different from that of the “Kickoff” Meeting on November 28. This time, a representative from LLNL was present. With the exception of LANL, there was therefore one representative from each of the eleven national laboratories participating in the initiative (LANL had two). As the session began, Ed Joyce suggested that since all “Review of Activities thus far” had been covered in the morning session, that this could be skipped and thus jump right to drafts of the “Review and Discussion of Mission, Vision, and Capabilities” to allow more time for a discussion. Dean Waters agreed and prefaced the discussion with a short introduction.

Jumping the gun somewhat, there ensued a discussion among the laboratory representatives concerning confusion on interpreting the capability form mailed shortly before the meeting. They were not distributed. The one-page summaries for each laboratory prepared for the November 28 meeting were distributed. A discussion on the role of independent CFD software vendors produced no consensus. Next the draft Mission and Vision statements were discussed followed by the definitions and inclusion of Capabilities. Several action items were decided upon: LANL would redraft the “Mission, Vision, and Capabilities” statements by January 15, 1996. LANL would also revise the Capability template and send it out to the laboratory representatives to be completed by February 1, 1996.

At 3:30 PM, Dean Waters discussed possible templates for the proposed Multiphase Center. A generic Memorandum of Cooperation was distributed. In conclusion, Waters and John Cummings offered some tidbits of wisdom They stated that the center should have a critical mass, on the order of $20–100 million/year. Rich Valentin estimated that, on the basis of the one-page laboratory capability sheets, the existing aggregate spending on multiphase activities totaled about $50 million. Waters stated that the following items should be performed: (1) Get the capabilities on the World Wide Web. (2) Be truthful in the assessment of capabilities. (3) Modify the generic Memorandum of Cooperation. (4) Get the Center established then market it. Don't count on any NEW money right away.

The "Dallas Team" thought this could be accomplished in as early as four months. Their other comments were: Near-term opportunities should not be missed. Don't put forth capabilities which cannot be shared, e.g., weapons R&D. The Mission and Vision statements should be revised every five years. Approach DOE Energy Research (ER) and NSF to get universities involved. A January meeting (actually workshop) in New Orleans was mentioned as a good opportunity. Define the customers and the product. Get capabilities assessment and then develop the roadmap. Get broad-based DOE backing early. Get the laboratory directors aware of the initiative and get their approval.

I received the description of my role for the OIT funding from Brian Volintine for the Multiphase VTC from Ed Joyce after this meeting on Jan. 8, 1996. It was to be my responsibility to receive and tabulate the capabilities of the various laboratories. If more funds became available, I would perform a comprehensive review of university activities and capabilities relevant to the VTC. Such a document was put together for Canadian universities as well government institutions in Canada [7]. I received the revised Mission, Vision, and Capabilities Statements from Ed Joyce on January 18, 1996. I received the Capabilities template from him on January 29, 1996. He instructed all laboratory representatives to complete them and to send them to me by February 6, 1996. They would then be reviewed and distributed in Washington DC at a meeting scheduled for February 21, 1996 at the same place as the November 28 "Kickoff" Meeting, 655 15th St. NW. The first batch started to arrive February 6, 1996.

16.2.4 Third VTC Meeting February 21, 1996

This was the third and last meeting of the representatives of what by then was generically referred to as the Multiphase Virtual Technology Center (VTC). It was held in the same rented office building at 655 15th St., NW Suite 300, Washington, DC where the first VTC meeting was held on November 28, 1995. The meeting was steered by Ed Joyce who welcomed all attendees. This time there was an overhead projector and poster board. Accompanying him was Dan Butler. This time there were representatives from ten laboratories including LANL: INEL (John Collins), SNL (Art Ratzel), ANL (myself), ORNL (Cloyd Beasley), BNL (US Rohatgi), PNNL (Jim Fort), LBNL (Dave Dragnich), LLNL (S.-W. Kang), and METC (Tom O'Brien). Walter Fuchs of PETC was absent. Brian Volintine from DOE OIT also attended. Rich Valentin from ANL arrived at 12:00 noon as a representative of the "Dallas Team" to get a sense of what was transpiring.

The meeting was called to order at 8:45 AM. For representatives who had not attended the two previous VTC meetings, Ed Joyce briefly reviewed the progress to date. I passed out the very preliminary, partially edited collection of the one-page laboratory capability summaries submitted to me by the laboratory representatives which I assembled into a draft document shortly before the meeting. Absents were BNL's and LBNL's. Then, a discussion of the capabilities statements ensued. It was decided to streamline them by including parallel computation into numerical methods and advanced testbeds and data bases into experimental methods. The revised capabilities agreed to then read:

(1) Numerical methods for multiphase flow.
(2) Phenomenology and constitutive theory and modeling, e.g., include: turbulence and exchange.
(3) Experimental methods for multiphase flows—advanced diagnostics, advanced testbeds, facilities, and data bases.
(4) Multiphase flow applications.

Each laboratory was instructed to submit to me revised one-page summaries for each capability which would then compiled into a VTC capabilities document. Summaries for each section would then be prepared after all of the one-page summaries were collected. Next the Mission and Vision Statements were reviewed. Ed Joyce rewrote them and e-mailed them out the same day after the meeting. The revised Mission and Vision Statements were

Mission Statement

The VTC for Multiphase Computational Fluid Dynamics (CFD) integrates and develops the resources of Industry, Government, Academia and Professional Societies, to enable reliable analysis in multiphase CFD. This will be accomplished by a focused effort to obtain a fundamental understanding which will be used to solve problems crucial to Energy Conversion, Industrial Competitiveness, Environmental Remediation, and National Security.

Vision Statement

The VTC will bring Multiphase Computational Fluid Dynamics (CFD) into the realm of an Enabling Technology. As such, the VTC membership will have the capability to predict with confidence the performance of various multiphase systems. The performance prediction will be comprehensive in that its impact on the environment and on resources will be discernible. The primary means by which the VTC focus will be maintained is by the creation, support, and validation of a computer simulation capability for multidimensional, time-dependent problems in complex multiphase flows that arise in problems important to the VTC membership.

The following major action items were generated from the meeting. (1) I was to compile and edit the revised summaries by March 13, 1996. The format is to have four sections corresponding to the four capabilities, each containing each laboratory's capabilities (not all laboratories might have contributions to all sections). (2) Cloyd Beasley (ORNL) was to draft a generic memorandum of cooperation (MOC) and send it to Ed Joyce (LANL) as soon as possible. (3) Nominees for Acting VTC Director were to be sent to Ed Joyce.

Ed Joyce e-mailed the draft MOC containing the roadmap, role, mission, vision, and capabilities of the VTC to all laboratories on March 7 for comments.

He arranged a conference call which was made on March 8 to discuss these items with apparently all eleven laboratories represented, as well as Dean Waters, and Rich Valentin representing the "Dallas Team". This was an interesting experiment in "virtual" conferencing, was quite successful, but rambling (it lasted 1.5 h). Ed Joyce promised an action item of setting up an electronic bulletin board. Dean Waters made some nice comments praising the terrific job of assembling the components of the VTC. He highly recommended that some money flow into the center to really make it take off like the robotics VTC did. Dean Waters challenged the VTC on how to marshal the capabilities into a program that the nation needs. Ed Joyce then made a presentation to the Laboratory Coordinating Council on February 22, 1996 reviewing the progress made to date.

I reviewed the draft MOC in April 1996 and, as far as I could tell, it was finalized by June. It was to be a MOC among the collaborators: Argonne National Laboratory, Brookhaven National Laboratory, Idaho National Engineering Laboratory, Lawrence Berkeley National Laboratory, Lawrence Livermore National Laboratory, Los Alamos National Laboratory, Oak Ridge National Laboratory, Pacific Northwest National Laboratory, Pittsburgh Energy Technology Center, Morgantown Energy Technology Center, and Sandia National Laboratories for the DOE Virtual Technology Center for Multiphase Dynamics (VCMD). Note the change of name and acronym.

This was considered to be one of the single most important action items resulting from the meeting. However, it fell into limbo. It was supposed to have been circulated to the national laboratory directors for signature. In a telephone conversation on April 25, Ed Joyce told me that he thought that the neither Cloyd Beasly nor I recalled any such decision, and it certainly was not documented. Without a signed MOC specifically tailored for the VTCMD, it was not a legitimate entity. This document must describe how it functioned, how the directors and committees were chosen, and liaisons with other government agencies. The entire MOC is included in Appendix I for historical reasons.

After this meeting, I started put together a document called the National Laboratories' Capabilities Summaries for the Virtual Technology Center for the Investigation of Multiphase Dynamics. I collected the revised summaries as they arrived, edited them, and assembled them together. They dribbled in over the next few months, and I went back and forth with Ed Joyce, who assumed the title of Acting Director, concerning the format of the document and several of the laboratory participants to draft the texts for the four capability areas listed above. There is no record of any voting regarding the selection of the Acting Director nor how he was chosen. The suggestion to have two directors was ignored. A preliminary draft was ready on April 12. A more complete draft was produced from this preliminary version on September 30. It went through one more revision on October 18. The final draft dated December 2, 1996 was sent to Ed Joyce for publication. To my chagrin and dismay he published this version as a LANL report with him as the author [8]. I did all the drudge work, and he took all the credit with just a one line acknowledgment to me as having assisted in the compilation.

16.2.5 National Workshop on Computational Fluid Dynamics and Multiphase Flow Modeling October 30–31, 1996

I attended the DOE sponsored "National Workshop on Computational Fluid Dynamics and Multiphase Flow Modeling" held October 30–31, 1996 at the University of Maryland. It was at this meeting that the nearly final draft version of the capabilities document developed at the third VTC Meeting February 21, 1999 was ready for discussion by the participants. I assisted Tom O'Brien in planning the Gas/Solids breakout session. Everybody who was anybody in the area of CFD and multiphase flow attended this meeting, invited by Denise Swink, then the Deputy Assistant Director for Industrial Technologies at the DOE.

During January and February, 1997, I participated in the VTCMD teleconference calls to plan the poster for the 2nd Industrial Energy Efficiency Symposium & Expo, February 24–26, 1997 held in Arlington, VA. I also prepared some material for this poster and gave it to Bill Schertz for his review. I volunteered to assist in manning the VTCMD poster but did not go to the meeting.

Brian Volintine asked me to review the printed draft of the report. Technology Roadmap for Chemical Industries of the Future—Multiphase Fluid Dynamics, henceforth referred to as the "roadmap document", distributed at this Expo [9], and to compare it with the electronic version distributed before the Expo by Ed Joyce in February to the national laboratory representatives of the VTCMD for comments. Except for formatting differences, I determined that the electronic version was identical to the printed version of the text in the printed report [9]. This document was a description of what was accomplished at the University of Maryland meeting October 30–31, 1996. The Executive Summary stated, "This report outlines the future technology needs of the Chemical Industry, in the area of Computational Fluid Dynamics and Multiphase Flow. Industry need in this area was highlighted in the recently published document Technology Vision 2020" [2]. The appendices contained collection copies of presentations made at this meeting.

In my review, I stated that as the document then stood, it was entirely too sketchy to assist the Vision 2020 team to use in the preparation of the Chemical Industry, Multiphase Dynamics RFP scheduled to come out in July 1997. I started to modify the text, and a coarse revision was prepared. Because there were such an extraordinary number of typographical and grammatical errors as well as inconsistent usages, I stopped. I only noted the major recommended changes and modifications. I sent my comments to Brian Volintine and Ed Joyce on March 23.

On March 24, Tom O'Brien returned my phone calls placed the previous week to discuss what happened at the 2nd Industrial Energy Efficiency Symposium & Expo. He stated that he was not certain whether the roadmap document should be just minutes of the National Workshop on Computational Fluid Dynamics and Multiphase Flow Modeling or whether it should be more substantial. Tom O'Brien and Jim Fort of PNNL had revised the rough draft of the roadmap document of February 12, 1997. They significantly expanded the description of Tables I and II containing priorities and time tables for gas/solids/liquid and gas/solids flow systems and inserted a discussion of multiphase turbulence. I reviewed this revision and sent comments back to Tom O'Brien, Ed Joyce and Brian Volintine on March 24, 1997. In this review, I questioned whether Brian Volintine or Ed Joyce wanted specific project descriptions in the document or just a straight reporting of the National Workshop on Computational Fluid Dynamics and Multiphase Flow Modeling with amplifications of Tables I and II. I suggested that the definitions of the three capability areas could be lifted from the capabilities document [8] and inserted into the roadmap document. I thought that this is basically what both Tom and Jim had paraphrased.

On March 27, I received the revised draft from Ed Joyce with the comment "… this is a live document that I am sure it will be updated as needed." Most of the copies of presentation materials in the printed rough draft [9] were removed. Subsequently I received another copy of the revised draft in PDF format from Brian VanderHeyden. This draft contained some of my suggestions but not my suggested revisions to the textual problems I had with the descriptions of Tables I and II nor a discussion of fine particle laminarization in risers. Appendix I contained Tyler Thompson's presentation National Collaboration on Multiphase Flow Modeling and comments on Research Needs for Math Modeling of Gas–Particle Systems by Ray Cocco, Bruce Hook, and Jon Siddall from Dow Chemical. Appendix II contained Grand Challenge Multiphase Flow Applications of Interest to DuPont by Kostas Kontomaris from DuPont. Appendix III contained National Laboratory Capabilities in the Virtual Technology Center for Multiphase Dynamics taken from "National Laboratories' Capabilities Summaries for the DOE Virtual Center for Multiphase Dynamics (VCMD)" [8] and Appendix IV contained University Perspectives documents from Sankaran Sunaresan from Princeton University and Clayton Crowe from Washington State University. Appendix V contained Summary of First Engineering Foundation Conference on Computational Fluid Dynamics in Chemical Reaction Engineering (CFD in CRE) by Milorad Dudukovic from Washington University, and Appendix VI contained a list of attendees with mailing and email addresses. Anyone wanting what appears to be the final PDF version of the roadmap document may try to contact Brian VanderHeyden at LANL or me. This document was substantially revised and streamlined and published in 1999 with a forward by Tyler Thompson and Konstantinos Kontomaris [10].

16.3 The Four-Year Multiphase Fluid Dynamics Research Consortium (MFDRC) is Formed

I was working with Fluent, Inc., Dow Corning Corp., and IIT on a revision of a NIST Advanced Technology Program (ATP) proposal which was submitted by Dow Corning in 1996 but failed to be funded even though we were a semifinalist. The NIST review of this proposal was used to substantially improve upon it. This was actually the second time that I had worked with Dow Corning on a NIST proposal. In 1995, I had worked with my colleague Jacques Bouillard and Michael Engelmann, president of Fluid Dynamics International, Inc. (FDI) then headquartered in Evanston, IL on a proposal titled Advanced Fine Powder Chemical Catalytic Processing Technology. FDI licensed the single-phase FIDAP finite element computer program and was later bought by Fluent, Inc. We proposed to integrate the solution scheme from the two-phase FORCE2 computer program discussed in Chap. 13.1 into FIDAP and commercialize the product. Unfortunately, the business plan was not very well developed, and the proposal was rejected.

The proposal titled Multiphase Fluidization Model for Fine Powders was submitted to NIST on March 17, 1997. This NIST proposal was quite similar in detail to the proposal I was working on in anticipation of the July 1997 DOE OIT Chemical Industry, Multiphase Dynamics RFP. The purpose of the NIST proposal was to develop a validated model for cohesive fine powders, called Geldart Group C, which would be incorporated into the commercial FLUENT computer program. We were informed on May 30 that once again our proposal was a semifinalist. An oral review of the proposal was to take place at NIST headquarters in Gaithersburg, Maryland on June 10. This was indeed a very good sign as it meant that the proposal had a very good chance of being accepted since two-thirds of semifinalists are funded. Dimitri and I flew together to Washington on June 9 and were met the next morning at NIST by, Peter Rundstadler from Fluent, Inc., and Sue Gelderbloom and Ward Collins from Dow Corning. Jim Chittick, Vice President of Manufacturing at Dow Corning, arrived separately via the corporate airplane. Sue, Peter, Dimitri, and I were the ones on the stage set up for questioning.

After the ten-minute introductory remarks by Sue and Dimitri, the questions started with the technical plan. Dr. Ron Davis was concerned that if Task 7 (Constitutive Relationships for Fine Powders) was not successful, we might not get to Task 14 (Heat Transfer). Sue walked through the return versus risk viewgraph for Geldart Group A, B, and C powders. Then Davis wanted to know how empiricism enters into the model. Dimitri explained how the effective restitution coefficient enters into viscosity, and the solids equation of state. Then, he wanted to know how the heat transfer enters. Gidaspow to the rescue again saying it affects density and hence bubble sizes. Dimitri handled almost all the technical questions. A question asked several times was how confident were we in the plan. I walked through the return versus risk viewgraph again.

At 1:35 PM questions shifted to the business plan. Questions here were: what is the level of confidence that for-profit companies would use the technology, how will the code be used, what happens if there was no ATP funding, how difficult is the parallelization to implement with multiphase, on what platforms will the code be used (last two questions from Ron Davis again), and since Dimitri was such an important link in the project, why was he in for only ten percent of his time. I stepped in and said we would share pre- and postdoctoral students as we have in the past. One question was significant: since we are all strong personalities, who is in charge. Sue immediately chirped up “I am.” Then, there were questions as to whether the ANL matching could be counted as in kind and whether Tasks 23 and

24 might be tossed out since they looked like commercialization tasks. Ward and Peter handled most of the questions, and Ward said if ANL could not supply match funds, that Dow Corning would find some more. Upon leaving after the review, the woman in charge of grants handed Ward Collins an information package concerning budget questions. It looked like we had made it and that the proposal would be funded.

The DOE OIT Chemical Industry, Multiphase Dynamics RFP was issued in July 1997 patterned after the solicitation No. DE-SC02-97-CH10885 Energy and Waste Minimization Research Supportive of Technology Vision 2020: The Chemical Industry. The three categories Numerical Methods, Phenomenology and Constitutive Relations, and Experimental Validation were to be considered in the proposal. The NIST decision after the oral review on June 10 dragged on over the next several months. The pre-application I was working on had to be sent to Brian Volintine by October 14, 1997. The proposals were to be sent to him by January 5 (extended to January 14), 1998. Only DOE national laboratories were allowed to apply. Approval for funding via the DOE FWPs would take place around March 1998. As far as I know there were only three proposals submitted. They were: (1) A Research Consortium for Multiphase Fluid Dynamics: Simulating Industrial-Scale Turbulent Gas-Sold Flows submitted by LANL, SNL, and PNNL with Dow Chemical as the lead supporting organization and a host of others. (2) Computational Fluid Dynamics for Multiphase Flow as Applied to Spouted Beds of Fine Particles submitted by FETC and LBL in collaboration with Fluent, Inc., and Dow Corning Corp. (3) Phenomenology and Constitutive Relations for Fine Powder Rheology in Riser Reactors submitted by ANL in collaboration with ORNL, Fluent, Inc., EXXON Research and Engineering Company, and IIT. The purpose of our DOE proposal was similar to the NIST proposal in that it was to produce a multiphase fluid dynamics model for fine powder rheology in riser reactors that would allow the chemical industry to optimize fine powder fluid–solids reactors. The strategy was to hedge our bets that if one of the two proposals would fail, perhaps the other would succeed.

Unfortunately, the politics of science once again reared its ugly head. LANL, with Dow Chemical as the lead supporting organization via Tyler Thompson, had already "been in bed" with each other to prepare their consortium proposal with the assumption that they would be the winners.

A meeting was held at IIT on October 5, 1997 to discuss the status of the LANL proposal in response to the OIT Chemical Multiphase CFD RFP. Present were Tyler Thompson, Dow Chemical, Susan Gelderbloom, Dow Corning, Dimitri, IIT, Richard Doctor and me, ANL. This meeting was a follow-up of a telephone conference call on September 30 involving the planners of the ANL proposal. In short, Thompson dealt ANL out since he had developed a five-year consortium plan whereby the Westinghouse cold model riser facility would be moved to SNL. He was asking for an initial total of $1,000,000/yr with $500,000/yr going to Sandia to instrument and operate the facility, $350,000/yr going to LANL for modeling support using the CFDLIB code, and $150,000/yr going to PNNL for acoustic measurements of density. CFDLIB was the code of choice even though it was in Tyler's opinion, "user unfriendly". Fluent, Inc. might come into the consortium later using their own funds to vend it. Other chemical industry participants involved in the proposed consortium in addition to LANL, SNL and PNNL were to be Dow Corning, DuPont Central Research and Development, Westinghouse Electric Corporation, Cray/SGI, Inc. Chevron Research & Technology Company and Exxon Research and Engineering Company. Universities involved were to be Clarkson, Purdue, Princeton, and IIT, all of which would be funded by cash in kind contributions from industry amounting to about $200,000/yr (approximately $50,000/yr each).

In a nice way, Tyler told the ANL team that they were free to submit their own proposal which would be complementary, but that the team he organized constituted persons and organizations familiar to Dow Chemical and with whose companies they have been dealing with "for some time." The exclusion of Fluent, Inc., ANL, and ORNL was deemed by Tyler to be "unfortunate" but was based on the assumption that our NIST ATP proposal then still under review would be funded and would complement the LANL proposal. It was also predicated on the perceived constraint that there was only going to be initially $1,000,000/yr from DOE OIT. Richard Doctor informed Tyler that having $850,000/yr going to New Mexico would not sit well with DOE to which Tyler responded that is a chance they would have to take.

In a telephone follow-up on October 6, George Cody of EXXON R&D told me he still supported the ANL proposal and that Peter Runstadler of Fluent, Inc. would participate. Details of Fluent, Inc's in kind contribution, cash needs (if any), and tasks would be discussed on Thursday October 9. The major tasks would revolve around putting the evolving improved constitutive relationships for cohesive powders into the FLUENT code. This would complement a Cooperative Research and Development Agreement (CRADA) just signed between Fluent, Inc. and FETC, wherein FLUENT, CFDLIB, and FETC's MFIX codes would be benchmarking two-phase problems of various kinds. A workshop was being held October 7 and 8, 1997 as a part of this CRADA. Tyler Thompson will be attending this workshop and talking with Tom O'Brien. Peter Runstadler said that Tyler was going to visit Fluent, Inc. later this month. Tyler was also going to present his proposal at the 9th CFCFD Users Group Meeting at Dow Corning/Dow Chemical, Oct. 16–17, 1997. The pre-application for the ANL proposal was sent to Brian Volintine by October 14, 1997.

Sue Gelderbloom was informed via telephone on October 10 that our NIST proposal was accepted. Then, later in the day NIST called back to inform her that it was not! A telephone conference call debriefing was held on October 21. The essence of the debriefing now follows. The proposal was "fundable" and had lots of positive comments, but there was just not enough money available to fund it. It was felt that technically the proposal addressed an important research area having a good team of expertise. The business plan was excellent with a wide dissemination of technology by Fluent, Inc. The fact that metrics are difficult for this type of project was not an issue. The ANL FWP for the DOE OIT RFP was mailed to Brian Volintine on January 14, 1998, just under the deadline.

Well, the ANL proposal was rejected as we expected it would be. The LANL proposal became the template for the DOE OIT Project, spearheaded by Tyler

Thompson with the FETC proposal shoehorned in. What happened to the Virtual Center for Multiphase Dynamics (VCMD) after all that planning with all of the national laboratories participating discussed above? It just silently morphed into this new consortium. What happened to the Mission, the Vision, the Memorandum of Cooperation, the Capabilities document [8], the Roadmap [9, 10]? All of this just disappeared as though it never took place. All the other national laboratories just vanished from the consortium. It no longer resembled a national program but a regional one resembling but superior to the one that Bill Sha tried to establish with the Multiphase Flow Research Institute (MFRI) discussed in Chap. 15.

The consortium was organized into Group A and Group C (by Tyler Thompson and perhaps Brian Volintine) standing (as an in joke of sorts) for Geldart Group A and Group C particles. Group A pretty much looked like the LANL proposal with LANL, SNL, PNNL Princeton University, Purdue University, Washington University, University of Colorado, and IIT as major players. The objective of Group A was to develop and disseminate a general, experimentally validated model for turbulent multiphase fluid dynamics suitable for engineering design purposes in industrial-scale applications of relevance to the chemical industry. The initial work was to focus on the particular case of a turbulent flow of a particle-laden gas at industrial conditions, especially as found in riser reactors and pneumatic conveying. Group A was focused on circulating fluidized beds having Geldart Group A particles (aeratable particles about 100 microns in diameter) similar to, and including, FCC catalyst.

Group C consisted of LBNL, ORNL, FETC, and IIT. The objective of Group C was to address (1) the cohesive behavior of Geldart Group C particles in the range of 10 microns in diameter, (2) a continuum description of the granular stress law in the dense, frictional flow regime, (3) coupling of heterogenous chemical kinetics with heat and mass transfer, (4) the long computational time required for transient simulations, and (5) subgrid-scale phenomena, such as particle clustering by using multiphase computational fluid dynamics capabilities which can be used to realistically simulate the dynamic behavior of a reactive, spouting bed of small particles.

The first meeting of the entire consortium was called the DOE/Chemical Industry CFD Project Kickoff and was held in Eagen, Minnesota at SGI Cray Research Park, July 20–21, 1998 and attended by 39 participants. The following is a synopsis of what transpired at this kickoff meeting. Ray Cocco started the meeting at 7:30 am and explained its purpose, i.e., to have a clear understanding of the two years of effort ahead and to develop a plan for the "big picture." Ray would become the ad hoc leader of the consortium meetings. The three DOE OIT representatives present were: Brian Volintine, Bruce Cranford, and Douglas Kaempf. Bruce Cranford was silent the entire meeting. The first day was recorded by a camcorder crew but no one mentioned what for and why. I still have these recordings on VHS tape in my possession. According to Tyler Thompson, Groups A and C started July 1 and the funding would be $2,000,000 for 15 months corresponding to the rest of DOE FY 1998 and all of FY 1999. The FETC/LBNL/ORNL project team was to receive $300,000 in each of 2 years for a total of $600,000. This included $25,000/yr for a total of $50,000 for little old me funded entirely independently to ANL by Brian Volintine by a separate FWP. Although neither I (nor ANL) were a part of the consortium, Tom O'Brien leader of Group C considered me to be a part of it. My role was a minor one, and I think I was viewed as a sort of intruder. The rest of the money went to the SNL/LANL/PNNL team in Group A. This allowed for a "full burn rate." Thompson assumed that DOE OIT would not walk away after 15 months and fully expected another $1,000,000 for FY 2000 so that they could have a "full burn rate" for 22 months. The two technical people from FETC (actually EG&G Technical Services West Virginia, Inc.) including Madhava Syamlal were leaving effective July 24 and hired by Fluent, Inc. to set up a field office across the street from FETC headquarters in Morgantown. The official name for the combined Groups A and C was voted on to be the Multiphase Fluid Dynamics Research Consortium (MFDRC). The inclusion of the word Computational was voted down. The consortium planed to have a booth at the February DOE/OIT Symposium & Expo. There would be a CFDLIB Workshop at LANL early in 1999. There would be a meeting of the modelers in Chicago at IIT in the fall to discuss turbulence modeling and the best Particulate Solid Research, Inc. (PSRI) data sets to model. Also to be discussed will be the various models in IIT Code, MFIX, and CFDLIB.

This so-called Modeling Meeting was held October 6, 1998 at IIT with Dimitri presiding and the Chemical Engineering Department hosting the event. The meeting was well attended with members of the MFDRC from LANL, FETC, SNL, ANL, Dow Chemical, Dow Corning, Fluent, Inc., Purdue University, and Exxon. There were guests from Universal Oil Products UOP (now Honeywell UOP) in Des Plains, IL, the University of West Virginia, and faculty and students from the Chemical Engineering Department. Five 20-minute presentations were followed by a presentation on modeling test cases. Extended discussions were then held on modeling theory. A discussion on experiments addressed what was needed for experimental input and what experiments were needed for model verification and differentiation between models. All in all, this informal meeting was quite successful and served to engage the principal computer modelers and experimentalists in a constructive dialog.

The MFDRC continued for roughly five years from July 1998 to September 2003. Besides the kickoff meeting and the "Modelers Meeting" there were to be seven more meetings of the full consortium: Wilmington, DE, September 26–28, 1999 (DuPont), Albuquerque, NM, April 12–14, 2000 (Sandia), Midland, MI, October 16–17, 2000 (Dow, Dow Corning), Morgantown, WV, April 17–18, 2001 (NETL), Salt Lake City, UT, August 29–30, 2001 (University of Utah), West Lafayette, IN, April 22–24, 2002 (Purdue University), and the last one in Columbia, MD, September 30–October 2, 2002 (Millenium Chemicals). There were also presentations for the MFDRC DOE OIT Symposium Progress Report by some members of MFDRC members at the DOE OIT Symposium & Expo in Washington DC on February 12, 1999. Group A would continue with the experiments on the SNL riser well into 2003 with a final report being issued as late as 2006 [11]. This report gives a summary of the MFDRC in the Executive Summary and Introduction. Reference [12] contained the following summary for the MFDRC in 2002 probably written by Tyler Thompson.

16.4 Vision 2020 Contributes to Commercial Success

16.4.1 Collaboration Pays Off—MFDRC Pushes the Frontier of Modeling of Materials Transport

The Multiphase Fluid Dynamics Research Consortium (MFDRC) was established in 1998 in response to priority research needs identified in the Vision 2020 *Computational Fluid Dynamics Roadmap*. To better understand and model multiphase flows, consortium members joined together to support learning and fundamental research. This partnership in basic engineering science will have broad impacts on chemical industry processing and future products. Members include ChevronTexaco, Dow Chemical, Dow Corning, DuPont, ExxonMobil, and Millennium Chemicals, the engineering software companies Fluent and AEA Technology, seven universities, and six national laboratories. R&D is jointly funded by the DOE Office of Energy Efficiency & Renewable Energy, DOE Office of Fossil Energy, the National Science Foundation, and participating companies.

Results as of 2002:

- Improved CFD software programs and capabilities derived in part from MFDRC results are now available from the national laboratories and the commercial developers Fluent and AEA.
- New insight into material flows has been achieved through the development of two alternative modeling techniques.
- MFDRC is developing a scientific community. A preeminent network of research specialists including company engineers has had a vital forum for sharing problems and insights and stimulating new ideas. Twenty-two young scientists at the graduate and postdoctoral levels have been trained in multiphase flows, expanding the talent pool required by industry to make use of this complex new field of computation. Effective teams have been fostered across many different academic departments and disciplines at universities and national laboratories. In total, more than 200 professionals have participated.
- Novel models validated by data from the consortium's experimental testbed and incorporated in the commercial programs are expected in three to five years. The commercial impact in chemical manufacturing will ultimately be realized in full-scale commercial plants and products designed and optimized using MFDRC results.

In the above summary the Vision 2020 *Computational Fluid Dynamics Roadmap* reference must be reference [10]. In my opinion, the story is highly overblown. At the MFDRC Review Meeting in Midland, MI, at Dow Chemical, October 16–17, 2000, Brian Valentine stated that the MFDRC was a model of how National Laboratories can work with industry and universities. He thanked the input from the MFDRC members who supplied him with materials for his course on multiphase flow at the University of Maryland.

Although much progress was made, very few of the research needs for multiphase CFD contained in the roadmap document [10] were met especially the development of a reliable and validated multiphase CFD code useful for industry. There were fundamental flaws in the makeup and operation of the MFDRC. It was clear from the start in my mind that there was a mismatch between Groups A and C. Group A was pushing LANL's CFDLIB code, and Group C was pushing FETC's MFIX code. There was no organized effort to validate either of these two codes either with the data that were being taken for the riser facility at SNL or by the university investigators. There was no one to lead such an effort. Results would be shown from each of the two codes demonstrating capabilities but with no coordination.

One software company that started attending the MFDRC meetings was CPFD Software, LLC located in Albuquerque, NM. CPFD licenses the Barracuda computer program developed by Dale Snyder, formerly from LANL. The CPFD stands for Computational Fluid–Particle Dynamics. Barracuda is a software package developed with industry to solve fluid–particle flow problems. Dale claims it to be every accurate since it treats particles correctly as discrete solids with true size distributions, not as a fluid, and runs extremely fast. Barracuda has been applied extensively in the chemical and petrochemical industries. Ray Cocco, who joined Particulate Solid Research, Inc. (PSRI) in Chicago after leaving Dow Chemical, and routinely uses Barracuda to simulate their experiments, told me that Barracuda was the code that resulted from the MFDRC effort. I was stunned.

Most of the consortium money went to transporting the Westinghouse cold model riser to SNL, modifying it, and equipping it with state-of-the-art non-invasive instruments. There was no real consortium leadership. Ray Cocco officiated at each of the meetings which consisted almost entirely of presentations by members of the MFDRC from the national laboratories, the universities, and the industrial partners as well as occasional invited guests. These presentations would then be followed near the end of each meeting by breakout sessions of the MFDRC participants to argue about how things were progressing, what should and could and could not be modeled and why. Groups A and C would present their reports and action items for the next MFDRC meeting. Then everyone would reassemble six months later to make another series of presentations as though there was no remembrance or recollection of the last meeting.

There were no Mission, or Vision statements, Memorandum of Cooperation, or explicit roadmap. Perhaps, it was implicitly assumed that these were in operation from the VCMD? Tasks identified in the DOE OIT RFP for LANL and FETC were followed independently with no coordination. The major reason for this sad situation was because there was no steering committee with a strong leader to do so or to review progress and make decisions. Brian Volintine attended quite a few of the meetings but never asserted himself. There was no reporting until Paul Sheihing, a more forceful and outspoken person from DOE OIT who eventually took over from Brian, brought up the issue of reporting requirements at the MFDRC meetings at SNL held in Albuquerque in April 2000. SNL then began issuing quarterly reports that did not start until the third quarter of 2001. These were not issued as official SNL reports and were sent to the MFDRC participants and DOE OIT.

Starting with the kickoff meeting in July 1998, and continuing until December 2000, I had been independently reporting quarterly to Brian Volintine summarizing the meetings which I attended and documenting, as best I could, stories concerning the return on investment (ROI) for CFD modeling in the chemical industry. It was Paul Sheihing who unilaterally canceled my work for Brian in 2001. The purpose of this task was to document industrial case studies of a non-proprietary nature that would clearly demonstrate the ROI of CFD modeling which would help the DOE OIT to justify present and future funding of the MFDRC in particular and multiphase CFD in general. In addition, it would benefit the awardees of proposed projects. The return should not only include the cost of the software, but also the engineer's time to set up the problem, perform the computations, analyze the results, and generate cost savings and/or productivity gains based on insights generated. A large addition to the ROI accrues if a pilot plant step or large-scale experimental facilities can be eliminated and/or reduced.

The general perception is that the ROI of multiphase CFD modeling in the chemical industry is significant, a factor of ten and up. As willing as the CFD community is to agree on the usefulness of the tool, chemical companies are extremely reluctant to share any dollar amounts saved from direct insight gained from using CFD simulations because of the highly competitive nature of the industry. Even stating the dollars saved by CFD modeling already gives away some information concerning the company's cost structure and overhead, and in general, the cost of doing business. Today it is not uncommon for software companies to showcase "success stories" some of which indicate "savings" but not necessarily the ROI.

In one of my quarterly reports to Brian Volintine I developed a template for ROI based on an open literature success story. It contains my own cost assumptions for the year 1998.

16.5 Return on Investment Template

Case Study No 1

Company		Precision Combustion, Inc.
Project		Gas Turbine Combustor Optimization
Source		Ref. [13]
Cost basis	Staff	$200 k/yr (fully loaded)
	CFD license	$20 k/yr (medium size company)
	Startup cost	$100 k amortized over 4 years ($25 k/yr)
	Equipment	$10 k workstation amortized over 2 years ($5 k/yr assuming zero salvage value)
	M&S	$15 k/yr (includes secretarial, report preparation, travel)

Simulation effort	1 month
Simulation cost	(k)
Staff	$16.67 k
Equipment	0.4
Startup cost	2.1
License	1.67
M&S	1.26
Total	$22.1 k

This is roughly the estimated cost reported in Ref. [13]

Cost savings	$200 k [13]
Type of savings	Elimination of testing
ROI	$200 k/$22.1 k = 9.05

In the above analysis $1 k = $1000.

One useful item produced by the MFDRC was a website. A preliminary web page was prepared by Ray Cocco and placed on the web site for the Chemical Process CFD (CPCFD) User Group at www.cpcfd.org. This web page was initially maintained by Dick LaRoche at DuPont and physically resided at SGI (Dick's former employer) on one of their servers. I volunteered to look into the possibility of having this web site on one of ANL's servers which are all highly secure. I talked with the web master for ANL's Energy Systems Division and he agreed to set up the web site. The server would be gratis, and there would be an up front set up charge and a small monthly maintenance cost that would come out of the project funding.

A telephone conference call was held on January 17, 2000, in which Renee Nault and Betty Waterman, from ANL's Information and Publishing Division, Tyler Thompson and Ray Cocco, and Richard Doctor and I, participated. A plan consisting of two phases was developed.

Phase 1 included the following items: (1) Argonne would install the MFDRC site at http://mfdrc.anl.gov. (2) All files will be transferred to Betty Waterman from Ray Cocco via CD-ROM. (3) All non-Argonne publications would require a signed copyright permission statement before they are posted on the web site. (4) The files were beta-tested on IPD's internal access-only development server before being placed on the public-access production server for review. (5) Once the site has been cleared, it was opened to the public.

Phase 2 included the following items: (1) All new content will be sent to Betty through and Ray Cocco and me, who also obtain copyright permission statements. Preferred were PowerPoint files, word-processing files, and photographs for reproducing them on the web site. (2) Pass worded, members—only area was set up. (3) Other future possibilities include online conference registration, membership applications, and other forms.

A cost and time estimate was made after the all the files referred to above were received. The estimated costs were found to be bearable considering the limited funding for the project and go ahead was approved. The reworked beta web site was set up for internal ANL review on February 22, 2000. Suggestions were incorporated into the beta web site on March 3, 2000. The issue of the domain name and other legal issues were discussed with Helen Cordell from ANL's Legal Division. She advised not to use an.org domain name because of red tape and excessive time delay to get this done through Argonne channels. We could use any.gov domain name, e.g., mfdrc.gov and/or gas-solids.gov, without any problem and this is what was recommended. The objective was to try to get the web site functioning in time to roll it out at the next MFDRC meeting at SNL in Albuquerque, April 11–14, 2000. The beta web site was moved from ANL's Information and Publishing Division internal development server to their public server on April 7, 2000. The site name adopted and hosted by ANL was http://mfdrc.anl.gov. Files received from Ray Cocco were recoded and restructured so that they would be faster loading and compatible with different browsers. A "research" area containing information about the research Groups A and C was added. New pages for a calendar, site map, and external links were added. The existing graphics design was modified to reflect these structural changes. Either Tyler Thompson or Ray Cocco wrote the mission and vision statements and were moved to the "overview" area. These statements differed significantly from these for the VCMD. They were:

MFDRC Mission Statement

By using statistically significant data from experiments based on large-scale unit operations, we will discern and validate the physics involved in modeling gas-solids hydrodynamics as applied to industrial problems. By unifying research efforts from the academic community, industry, and national laboratories, we will be able to approach this problem in an efficient and cohesive manner.

MFDRC Vision Statement

Commercially available computational fluid dynamics codes have the validated features to model all aspects of industrially relevant gas-solid hydrodynamics. The results of using these codes will save hundred of millions of dollars in capital and millions of BTU/year in energy consumption.

My opinion is that they were very weak. I assisted Ray Cocco when he presented the MFDRC web site at the MFDRC Review Meeting at SNL. I have a copy of the web site CD ROM as it stood at this point in time. The MFDRC web site subsequently continued to be maintained and updated over the life of the MFDRC.

In closing, I can only say that the MFDRC never had nearly the national attention that the National Technology Initiative received [14]. It was only because Vice President Al Gore, a technically savvy person, was convinced of its viability and impact that it took off. That initiative is a model that should be followed if there is ever going to be an attempt to have a National Multiphase Computational Fluid Dynamics Initiative. With the current administration under President Donald Trump, the likelihood of this happening is precisely zero. In addition, the planned merger of Dow Chemical with DuPont and the return of Dow Corning into Dow Chemical concomitant with the elimination of DuPont's entire research staff does not auger well for the US Chemical industry in the twenty-first Century.

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Chapter 17
NETL Initiates Workshops on Multiphase Flow Research Later Called Multiphase Flow Science

As I described in Chap. 13, Madhava Syamlal together with Tom O'Brien (and me indirectly) initiated NETL's MFIX open-source computer program. It continues to be improved over the years adding features which would later be incorporated into the FLUENT code. The basic documentation for theory, users manual, and numerics [1–3] was published in the 1990's. Hard on the heels upon the disbanding of the MFDRC in 2004, or 2006 if one considers the time to document the riser experiments at SNL [4], NETL began an annual workshop on multiphase flow. The first one in 2006 was called the Workshop on Multiphase Flow Research and was held at NETL June 6–7, 2006.

Researchers from universities, industry, national labs, NASA, and NSF met to discuss outstanding research problems in multiphase flow with particular relevance to energy technologies, and to chart out a roadmap for solving those problems. Attendance was by invitation only, and the meeting was not open to the public. Participants also included collaborators which NETL was funding, for a total of 79 including METC staff. The participants at this first workshop included a goodly number of those who had participated in the MFDRC described in Chap. 16. The vision of the workshop was to "ensure that by 2015 multiphase science-based computer simulations play a significant role in the design, operation, and troubleshooting of multiphase flow devices in fossil fuel processing plants." The discussions were organized into four technical tracks: (1) dense gas-solids flows and granular flows, (2) dilute gas-solids flows, (3) liquid-solids/gas-liquid flows, and (4) computational physics and applications. The outcome of this workshop was a document which I will refer to as the multiphase roadmap [5]. After an absence of 3 years, the second workshop was held at the Euro Suites Hotel in Morgantown, April 22–23, 2009. The name changed from Workshop on Multiphase Flow Research to Workshop on Multiphase Flow Science. These annual Workshops continue to the present day with the next one to be held August 8–10, 2017, in Morgantown.

As mentioned in the Preface, Madhava Syamlal assisted me in organizing two sessions at the AIChE Annual Meeting in Memphis Tennessee on November 11, 2009, titled Festschrift for Professor Gidaspow's 75th Birthday. These sessions

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honored our former teacher and Ph.D. thesis advisor at Illinois Institute of Technology. It was at this venue that Syamlal presented the paper Roadmapping of Computational Multiphase Flow [6]. It was from Syam's presentation that I learned of the Multiphase Roadmap [5]. I suggested to Syam that I might be able to assist him in his endeavor. In early February 2010, he informed me that NETL was planning to go ahead with the project and that a contract would be put in place. I received the contract and was brought on as an Independent Contractor because I was unemployed and not at ANL at the time. I then proceeded to prepare my presentation for inclusion at the 2010 Workshop on Multiphase Flow Science to be held at the Pittsburgh Airport Marriott Hotel, May 4–6 [7]. I met several times at PSRI in Chicago with Ron Breault from NETL and Ray Cocco, then Associate Technical Director, to go review my presentation and to finalize it. My presentation was given before the dinner the evening of the first day of the meeting.

After this workshop, I proceeded to prepare my report which was finished on June 6 and then sent to NETL. It was reviewed by Ron Breault who offered several constructive comments. I then submitted the revised report back to NETL. Neither my report nor my presentation was ever posted on the NETL web site for the Multiphase Flow Science Workshop in spite of my repeated inquiries.

I include this report, with minor typographical errors corrected, in Appendix J since it is available nowhere else and has not been published. I received permission from Syam to use it for this book. This report includes a review of the events which lead up the formation of the MFDRC and my assessment of its accomplishments. In effect this review constitutes thoughts and impressions formed not long after the dissolution of the MFDRC that are now more fully fleshed out in this book. When I prepared this report, I was much more upbeat, but as I wrote this book, I became less so because I perceived that it was a continuation of the politics of science which began in a state far away in Part 2. I review the Multiphase Roadmap report [5] in detail pointing out its deficiencies followed by recommendations for strengthening the roadmap. Three appendices include two proposed research areas not given enough priority in the roadmap report: erosion and dense suspension flow and ten questions, devised by Ron Breault, which were submitted to the attendees requesting their answers. Syam was the Focus Area Leader for Computational Science and Engineering from 2007. In 2015 he became Senior Fellow, Computational Engineering. In my opinion, the direction and content of the NETL Multiphase Science Workshops has declined considerably. It is not clear now who at NETL really decides what multiphase research areas to follow.

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Part V
Muliphase Conferences and Gidaspow's Books

Chapter 18
Conferences and Workshops Addressing Multiphase Needs and Problems Begin Due to Professor Dimitri Gidaspow's Initiatives

Conferences and workshops concentrating on multiphase flow started on the wake of Dimitri's 1974 Roundtable Discussion Modeling of Two-phase Flow, at the 5th International Heat Transfer Conference, Tokyo, Japan, September 3–7, 1974 [1]. A sampling of the more important ones is presented in this chapter. The 1975 ASME Winter Annual Meeting held November 30–December 4, in Houston, Texas, was where I presented the characteristics paper followed by its discussion and rebuttal. See Sect. 8.2 and Appendices D and E for details. This meeting was followed by the Two-Phase Flow and Heat Transfer Symposium-Workshop held in Fort Lauderdale, Florida, October 18–20, 1976. The papers were published in four volumes in 1978 by Hemisphere as Two-Phase Transport and Reactor Safety [2]. There were to be four more such conferences over the next 12 years held in Miami Beach, Florida. The next was the 2nd Multiphase Flow and Heat Transfer Symposium Workshop, held April 16–18, 1976, at which Brian Spalding chaired the Workshop on Mathematical Modeling and Computational Techniques. The thrust of this workshop was the issue of the ill-posedness of some two-phase equations and theorems concerning the characteristics of them. The next in the series was the 3rd held April 18–20, 1983. The 4th Miami International Symposium on Multi-Phase Transport and Particulate Phenomena was held December 15–17, 1986. This series ended with the 5th Miami International Symposium on Multiphase Transport & Particulate Phenomena held December 12–14, 1988. The proceedings were published in 1990 [3]. Then followed the NATO Advanced Study Institute on Two-Phase Flows and Heat Transfer August 16–27, 1976 held on the campus of the University of Bosphorus in Istanbul Turkey. There was a session on Suggestions for Further Research and Urgent Problems on Two-Phase Flows and Heat Transfer in which Dimitri and Charlie participated. The proceedings were published in three volumes in 1977 [4]. Dimitri played important roles in each of these meetings even though he did not attend the ASME Winter Annual Meeting in Houston.

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EPRI held a Workshop on Basic Two-Phase Modeling in Reactor Safety and Performance, in Tampa, Florida, February 27–March 2, 1979. The list of participants was a Who's Who of experts in all phases of two-phase flow research, including the late Brian Spalding. I was not invited, but Dan Hughes, still at EI, and Charlie and Vic Ransom from EG&G Idaho, were invited. In 1980 EPRI published the two-volume Proceedings [5]. In the early 1980s, Dimitri and I petitioned the AIChE to add the Multiphase Flow Area 7 g to the Heat Transfer and Energy Conversion Division (now the Energy Transport Division). This request was granted and subsequently many technical sessions were sponsored at the National Heat Transfer Conferences and AICHE meetings over the decades. Dimitri became the first chair of Multiphase Flow Area (7 g). I was next followed by fine string of able chairs. Dimitri is very proud of delivering the lecture for the Donald Q. Kern Award at the 23rd National Heat Transfer Conference on August 5, 1985. It was published in 1986 [6]. The AIChE Particle Technology Forum (PTF) was chartered in 1992 and became fully functional in 1993 with L.-S. Fan as its first Chair. The PTF is an international and interdisciplinary forum that promotes information exchange, scholarship, research, and education in the field of particle technology. The PTF sponsors a significant number of sessions at the AIChE Annual Meetings and has sponsors for the Lifetime Achievement and Thomas Baron Awards, both of which Dimitri has received. The PTF also participates in the World Congress on Particle Technology held every 4 years starting in 1990. The next one will be held in Orlando, Florida, April 22–28, 2018.

The first International Conference on Multiphase Flow (ICMF) was held in Tsukuba, Japan, in 1991. The second ICMF Conference was held in Kyoto, Japan, in 1995 where it was decided the conference should be held every 3 years. ICMF 1998 was held in Lyon, France, ICMF 2001 in New Orleans, ICMF 2004 in Yokohama, Japan, ICMF 2007 in Leipzig, Germany, ICMF 2010 in Tampa, sponsored by the University of Florida, ICMF 2013 in Jeju, South Korea, and ICMF 2016 in Firenze, Italy. The ICMF has become the largest and most important conference devoted to multiphase flow. The International Conference on Computational and Experimental Methods in Multiphase and Complex Flow is sponsored by Wessex Institute. The first conference in the series was held in Orlando (2001). It now alternates with the ICMF conferences. The next was held in Santa Fe, New Mexico (2003), followed by Portland, Maine (2005), Bologna, Italy (2007), New Forest, UK (2009), Kos, Greece (2011), A Caruna, Spain (2014), and Valencia, Spain (2015). The next meeting will be in Tallinn, Estonia, June 20–22, 2017.

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Chapter 19
Gidaspow Publishes His Two Multiphase Books

19.1 Multiphase Flow and Fluidization Continuum and Kinetic Theory Descriptions

Dimitri completed his first book (he started one on Greens Functions and one on Numerical Methods with Charlie in the late 1960s) subsequently referred to as MFF [1]. It summarizes over fifteen years of research at IIT and ANL up to 1992 in the areas of multiphase flow and fluidization. Dimitri and I were invited by Martin Welsh at the CSIRO in Melbourne, Australia, in 1993 to give lectures on fluidization. Dimitri used the galleys of his book to give his lectures, and I collected viewgraphs together from the METC Cooperative R & D Venture described in Sect. 13.1 to give mine. The course was given December 20–23, 1993. It was rather cool and rainy, but Dimitri wanted to go swimming in what he kept calling “the Tasmanian Sea.” Each morning, I would drive him to the beach near our hotel. Even though there were jelly fish floating in the surf, he would gingerly dive in and swim around for 15–20 min while I waited patiently on the beach. Then I would drive back to the hotel for him to change clothes after which we departed for CSIRO to gives the lectures. Dimitri and I arranged the lectures so that he could take a break while I delivered mine.

The research contained in MFF began in 1978 at LLL when Dimitri, Terry Galloway, and I collaboratively developed a step-by-step building-block hydrodynamic modeling approach to understanding the hydrodynamics of fluidized beds, closely coupled to validation experiments [2]. This work formed the basis of Dimitri’s response to a DOE University Program RFP. A two-year grant to study solids circulation around a jet in a fluidized bed was awarded to him in September 1978, thus initiating the research. Subsequent grants from the Gas Research Institute, the NSF, and a contract from Westinghouse Electric Corp. allowed the early work to continue and advance. The major interest at the time was synthetic fuels production using fluidized bed to gasify coal since this was in the era of the first serious US energy shortage caused by the Arab oil embargo. Progress was slow

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because the equations could generally only be solved numerically, and the running times on the computers at IIT were very long. Subsequent continuing support from the DOE, NSF, and industry allowed the research to continue, as has Dimitri's and my collaboration.

Multiphase flow and fluidization theory took a quantum leap with the appearance of MFF for which there was essentially no competition. Only Professor S. L. Soo's book [3] comes close; however, it is more broadly based and constitutes a textbook version of the classic monograph first published in 1967 [4] long out of print and subsequently revised in 1990 [5]. The kinetic theory is developed for fluid–solids with an emphasis on gas–solids fluidization and transport. In January 1986, Dimitri's 1984, Donald Q. Kern Award Lecture was published as the lead article in Applied Mechanics Reviews [6]. He considers this review to be the basis of MFF which then took the better part of ten years to complete. In the intervening years, the kinetic theory he developed for granular flow evolved into a viable adjunct to the continuum multiphase theory including fluidization. Dimitri's derivations and applications were the first time they appeared in such a textbook which is meant to be used as an advanced text in transport and fluidization courses as well as by industrial researchers. This section of my book constitutes a brief summary of my detailed review of MFF published in 1995 [7] to which I humbly recommend the reader. Since MFF's appearance, there have been over 3000 citations on Google Scholar and growing.

19.2 Computational Techniques: The Multiphase CFD Approach and Green Energy Technologies

Fifteen years after publishing his first book described above, Dimitri published his second book with his coauthor Veeraya Jiradilok [8]. Part I, Numerical Methods, and Part III Green's Functions and Functional Analysis contain his class notes developed in the Department of Gas Technology and later the Department of Chemical Engineering at IIT while teaching the two courses Numerical Methods and Transport Phenomena. Part II contains an update of his research since 1992, an exposition of the basic kinetic theory and its extension to the multiphase theory of mixtures, and a manual for the IIT code which Dimitri refers to as the Navier–Stokes solver. A CD-ROM contains the open-source versions of programs which Dimitri now utilizes in his Computational Techniques course. The material in the book has been used in the form of class notes taught to graduate and senior undergraduate students in chemical and mechanical engineering departments at IIT for the last four decades. The computer codes, particularly the Navier–Stokes equation solvers, have been developed by several Ph.D. students over the period since the appearance of his first book.

The theory of fluidization and multiphase flow is based on the new paradigm that emerged in the 1980s as granular flow [9]. Commercial CFD codes, such as

ANSYS FLUENT version 12.0 [10], contain Dimitri's extension of this theory described in his first book [1]. The programs described in this text [8] can be easily updated as new theory is developed because the open source of the basic IIT code versions is contained on the CD-ROM. For example, the codes can be extended to anisotropic and multisize particle flow based on the emerging kinetic theory [11]. Hence this book should be useful to research engineers in industry, to graduate students and to professors teaching a first course in computational techniques. The book illustrates how the IIT code as well as commercial CFD codes can be used for the design of green energy technology processes.

A basic understanding of numerical methods and the theory of ordinary and partial differential equations are necessary for successful CFD modeling. For example, some two-fluid models were found to be ill-posed as initial value problems and required changes to the basic physics to make them well posed as described in Sects. 6.1 and 7.3. Even with two-fluid equations that are well posed, a convergence study may not necessarily produce a grid size-independent solution. For example, in solving fluidized-bed heat transfer problems it becomes necessary to make the grid sizes for the energy equation much smaller than those for the flow, due to the large wall to bed heat transfer coefficients [12].

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Chapter 20
Conclusion—What Does the Future Hold?

This chapter offers the reader a historical summary with conclusions reached and some opinions/facts on where the technologies developed will be applied in the future and what, if any, improvements can or will be needed.

Well, it's been quite a trip from Dunkirk, New York, to Cleveland, Ohio, Chicago, Illinois, Idaho Falls, Idaho, Livermore, California, and back to Chicago and environs with many side trips in between all in a mere 60 years. First, I'm going to ramble a little bit.

As best I could, I have traced multiphase science and computational fluid dynamics (MSCFD) from its origins right up to the present. I feel lucky to have been thrust into this story by forces unknown to me which I have called predestination. There have been a lot of highs and a lot of lows, but on the average I feel highly privileged to have lived through the experience. The constant influence in my scholastic endeavors and professional career has been Dimitri Gidaspow whom I consider to be my mentor and guiding light. In order to honor him, I have organized no less than three Festschrifts for him for his sixty-fifth, seventy-fifth, and eightieth birthdays in three different venues: Albuquerque, New Mexico; Nashville, Tennessee; and Atlanta, Georgia. Plans are underway to honor him with another Festschrift for his eighty-fifth birthday in 2019. To him and his first student, Charlie Solbrig, this book is dedicated.

What I want to do to wrap up this book is to relate to the reader some of the lessons learned and to point out a few things that multiphase science can address in the future. Discussions with Dimitri helped me to crystallize my thoughts for this chapter. I have to emphatically remind the reader that multiphase science came about to better address the safety analysis of nuclear-powered reactors for the production of electricity for the public sector. Admiral Hyman Rickover who was responsible for building Nautilus, the world's first nuclear-powered submarine for the Navy in 1954, was a fanatic about safety. Westinghouse was chosen by Rickover to develop the pressurized water-cooled nuclear reactor for the Nautilus submarine which led to the development of nuclear reactors for commercial power production. More test reactors, including LOFT, were built in Idaho at the NRTS

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established back in 1949. Rickover had a powerful influence on his former aide, Milton Shaw, who became the director of the AEC Division of Reactor Development and Technology in 1964. He wholeheartedly embraced the necessity for nuclear reactor accident prevention because he had been exposed to the safety philosophy of the Nuclear Navy instilled by Rickover [1]. Hence, the development of computer programs for accident analysis for commercial nuclear reactors starting with RELAPSE-1 in 1966 [2].

As delineated in great detail in Chap. 4, Charlie Solbrig was responsible for developing an advanced two-phase model and convincing the AEC to initiate a program to develop a new computer program called SLOOP, which would improve the predictive capability of the single-phase computer programs then used for safety analysis. The politics of science discussed in Chap. 7 led to its demise in 1975. The overriding reason for its demise was the vituperative and destructive actions of L.S. Tong, Charlie's former supervisor at Westinghouse Electric. The other reason was the unforeseen computational difficulties associated with the discovery of the ill-posedness of the two-phase equations. As discussed in Chap. 9, several members, including me, left the SLOOP code program at ANC and went to Energy Incorporated to help develop RETRAN for EPRI. Vic Ransom stayed behind and pulled together the pieces developed for the SLOOP code project and, together with John Trapp and Dick Wagner, developed RELAP5 as discussed in Chap. 10. It turned into an international success. Another instance of the politics of science was Frank Harlow's copying Charlie's equations which lead to the development of the KACHINA, K-FIX, and TRAC computer codes at LASL. No credit was ever given to Charlie or to the SLOOP code program.

The energy crisis caused by the Arab oil embargo in the mid-1970s together with the dwindling supply of natural gas led to the need for the USA to produce synthetic fuels (synfuels) from abundant coal reserves. This is what motivated the DOE to fund Systems, Science and Software and JAYCOR to develop the computer programs CHEMFLUB and FLAG described in Chap. 11 to better understand the hydrodynamics of coal gasification in fluidized beds. Unfortunately, these efforts failed. The energy crisis is also what started Dimitri to have me get the K-FIX computer program from LASL and to begin the multiphase computer code development at IIT as described in Chap. 13. I was also instrumental in contributing to the initiation of the MFIX at NETL

While there are no obvious safety problems associated with synfuels production, (a coal gasifier might turn into a giant clinker which would have to be jackhammered out), there existed a sleeping giant in the US petroleum exploration and production industry which never perceived any need for safety analyses. Ever since the first oil strike in Titusville, Pennsylvania, in 1859, there have been safety consequences associated with drilling for oil both of an environmental and human nature. One might say that every uncontrolled gusher is an accident until it is brought under control. There have been hundreds maybe thousands of oil spills and blowouts but the petroleum business treats these as a part of doing business. That is until the really big one happened with the April 20, 2010, explosion on board the Deepwater Horizon drilling platform which led to an 87-day blowout of the

Macondo oil well nearly one mile deep in the Gulf of Mexico, known to everyone as the BP Oil Spill. Incredibly there were never any safety studies performed by the industry to deal with such a potential catastrophe. Instead they did risk analysis which is equivalent to playing Russian Roulette [3]. They should have been studying what amounts to the maximum credible hypothetical oil blowout (HOBO) accident. This blowout was the equivalent of either the hypothetical LOCA of a PWR or the meltdown of the fuel rods at Three Mile Island in 1979, studied in detail by the NRC. If BP staff had done a safety analysis and had a strategy in place, they might have avoided the blowout, or at the least contained it much more quickly. As it was there was no plan, and therefore, they didn't have any idea what to do. Following the tragic Piper Alpha incident in 1988, the UK established Safety Case Regulations (SCR) based on the recommendations from the official inquiry lead by Lord Cullen who stated "Primarily the safety case is a matter of ensuring that every company produces a formal safety assessment to assure itself that its operations are safe" [4]. What was initiated instead was a hurry-up study involving several US national laboratories including NETL to assess the flow rate of the BP blowout [5]. No detailed multiphase computations were performed. Dimitri was so outraged at this accident that he had the smarts to simulate this blowout on his own time and presented the results in a paper presented at an AIChE meeting which was later published [6].

There exists serious research in Italy into volcanology and in particular pyroclastic density currents (PDC) phenomena. Augusto Neri, one of Dimitri's former Ph.D. students, has recently been named director of the Volcanoes Research Department of the Istituto Nazionale di Geofisica e Vulcanologia (INGV) in Pisa, Italy. He is responsible for planning and coordination of volcano research work including modeling eruption dynamics with multidimensional and multiphase flow codes he developed and used for his doctoral dissertation. He reviewed the current and evolving state of knowledge of dangerous volcanic phenomenon and implications on the challenges for hazards mitigation [7]. Current efforts are aimed at estimating PDC hazard and risk, taking into account the relevant uncertainties. They represent an important step toward the long-term goal of developing an interdisciplinary and integrated approach to risk reduction. Such models are effective in representing the complex behavior of PDC phenomena and enable simulations that include remarkable detail of dynamic pressure and temperature, which can be used to quantify the expected hazard impacts.

I organized a team and tried valiantly several times to get funding from the National Institutes of Health (NIH) in the area of multiphase hemodynamics. In particular, our aims were to (1) develop the multiphase hemodynamic CFD model and experimentally validate it, (2) experimentally validate the combined multiphase CFD-monocyte adhesion model and perform sensitivity analysis of system parameters from the perspective of atherosclerosis initiation, and (3) evaluate the model's capabilities to predict areas of carotid artery atherosclerosis initiation in the clinical setting. The idea is quite easy to enunciate. First do an MRI scan of the area under consideration, say the carotid artery, generate the detailed computational mesh, perform the multiphase calculations, archive the result, and then use them to guide the diagnosis. This approach is meant to be proactive rather than reactive, that is, analyzing the conditions leading to the initiation of the disease and therefore taking action before it causes damage, thus requiring expensive treatment. Such procedures are already used in England to guide surgeries, but as far as I know not to any extent in the USA. After each review, we would respond to their comments, revise the proposal, and resubmit. Then the review committee would totally change and the reviews would be worse than before. We were never given a grant and gave up, frustrated. What we were proposing was apparently too novel. And we wound up educating these review committees. Worse yet, we were challenging some of the reviewers. We were able to publish several papers as a result of this effort which I believe will inspire future investigators to follow in our footsteps [8–11].

Finally, there is a need to establish a national initiative for MSCFD along the lines of the National Nanotechnology Initiative [12]. In Chap. 15 I went through the agonizing attempts to establish a national initiative for MSCFD. Bill Sha tried to establish his Multiphase Flow Research Institute (MFRI) at ANL in collaboration with Jim Hartnett from the Midwest Universities Energy Consortium, Inc. at the University of Illinois Chicago. It proved to be little more than Bill's attempt to rise above his long-time floundering attempt to develop the COMMIX-M code to be its director of the MFRI and to fund just two of his favorites from a field of many dozen applicants. Then in Chap. 16 I traced the tortuous path from the attempt to establish the Virtual Center for Multiphase Dynamics (VCMD) which led to the Multiphase Fluid Dynamics Research Consortium (MFDRC) for the chemical process industry which ended in roughly 2003. Today the sessions sponsored by the AIChE Particle Technology Forum established in 1992 and the Workshops on Multiphase Flow Science at NETL started in 2006 constitute the remnants for multiphase research in the USA.

Some of the areas of research I would include in a national multiphase initiative include:

1. Prediction of flow regimes for vapor–liquid flow similar to what has been done for fluid–solid flow [13].
2. A sound theoretical basis for the equations governing multiphase flow in porous media. We applied the so-called multiphase porous media model in the ANSYS FLUENT code [14] to model reactive distillation [15], but the theoretical basis is unjustified.
3. Extension of erosion modeling as proposed in Appendix J Review and Comments on the 2006 NETL Technology Roadmap Appendix A.
4. Analysis of dense suspension flow as proposed in Appendix J Review and Comments on the 2006 NETL Technology Roadmap Appendix B.
5. Improved models for boiling and condensation as reviewed by Kharangate and Mudawar [16].
6. Finally, I would include chaos and the resolution of the ill-posedness for one-dimensional two-phase flow modeling discussed in Chaps. 6, 7, and 8. These two subjects continue to be investigated to the present day [17].

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Appendices

Appendix A: Acronyms and Abbreviations

ACRS	Advisory Committee on Reactor Safeguards
AEC	US Atomic Energy Commission
AGA	American Gas Association
ANC	Aerojet Nuclear Company
ANL	Argonne National Laboratory
ANS	American Nuclear Society
ASME	American Society of Mechanical Engineers
ATHRP	Analytical Thermal Hydraulics Research Program
BES	Basic Energy Sciences
BNL	Brookhaven National Laboratory
BWR	Boiling Water Reactor
CFD	Computational Fluid Dynamics
CHF	Critical Heat Flux
CMT	Chemical and Materials Technology
CPCFD	Chemical Process CFD
CT	Components Technology
DC	District of Columbia
DOE	US Department of Energy
ECCS	Emergency Core Cooling System
EES	Energy and Environmental Systems
EI	Energy Incorporated
EPRI	Electric Power Research Institute
ERDA	Energy Research and Development Administration
ES	Energy Systems
EVET	Equal Velocity Equal Temperature
EVUT	Equal Velocity Unequal Temperature
FBC	Fluidized-Bed Combustion
FOPDE	First Order Partial Differential Equation
HEMM	Homogeneous Equilibrium Mixture Model
ICE	Implicit-Continuous-Fluid-Eulerian
I&EC	Industrial and Engineering Chemistry
IGT	Institute of Gas Technology

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IIT	Illinois Institute of Technology
INC	Idaho Nuclear Corporation
INCA	Idaho Nuclear Code Automation
INEEL	Idaho National and Engineering Laboratory
INEL	Idaho National Engineering Laboratory
INL	Idaho National Laboratory
JCP	Journal of Computational Physics
JFM	Journal of Fluid Mechanics
LANL	Los Alamos National Laboratory
LASL	Los Alamos Scientific Laboratory
LBL	Lawrence Berkeley Laboratory
LCC	Laboratory Coordinating Council
LLL	Lawrence Livermore Laboratory
LLNL	Lawrence Livermore National Laboratory
LOCA	Loss-of-Coolant Accident
LOFT	Loss of Fluid Test
MBO	Management by Objectives
METC	Morgantown Energy Technology Center
MFDRC	Multiphase Dynamics Research Consortium
MFRI	Multiphase Flow Research Institute
MIT	Massachusetts Institute of Technology
MOC	Method of Characteristics
MRI	Multiphase Research Institute
MUEC	Midwest Universities Energy Consortium, Inc.
NETL	National Energy Technology Laboratory
NIST	National Institute of Standards and Technology
NRC	US Nuclear Regulatory Commission
NRTS	National Reactor Testing Station
NSF	National Science Foundation
OIT	Office of Industrial Technology
ORNL	Oak Ridge National Laboratory
PDF	Partial Differential Equation
PETC	Pittsburgh Energy National Laboratory
PNL	Pacific Northwest Laboratory
PNNL	Pacific Northwest National Laboratory
PFP	Request for Proposals
PSRI	Particulate Solid Research, Inc.
PWR	Pressurized Water Reactor
RFP	Request for Proposal
RPI	Rensselaer Polytechnic Institute
ROI	Return on investment
RSR	Reactor Safety Research
SAI	Science Applications, Inc.
SCORE	Seriated Core

SLOOP	Seriate LOOP
SNL	Sandia National Laboratories
SSUVET	Steady-state unequal velocity equal temperature
SSUVUT	Steady-state unequal velocity unequal temperature
S^3	Systems, Science and Software
STUBE	Seriated Tube
TRSP	Thermal Reactor Safety Program
UCG	Underground Coal Gasification
US	United States
USA	United States of America
UVET	Unequal Velocity Equal Temperature
UVUT	Unequal Velocity Unequal Temperature
VCMD	Virtual Center for Multiphase Dynamics
VTC	Virtual Technology Center
WVU	West Virginia University
ZVUT	Zero Velocity Unequal Temperature

Appendix B: Herbert Kouts' 26th Water Reactor Safety Information Meeting Speech, 1998

HISTORY ON SAFETY RESEARCH PROGRAMS
AND
SOME LESSONS TO BE DRAWN FROM IT

PRESENTED AT THE 26TH WATER REACTOR SAFETY
INFORMATION MEETING
BETHESDA MARRIOTT HOTEL
OCTOBER 26-28, 1998

HERBERT JOHN CECIL KOUTS
BOARD MEMBER
DEFENSE NUCLEAR FACILITIES SAFETY BOARD
WASHINGTON, D.C.

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One of the benefits of passing years, if there are any benefits at all, is that one is then permitted to stand up in front of a group of younger people such as those here and tell how things happened before those people were around. In fact, there will even be occasions when there is a captive audience, such as this one. Even maybe an audience of younger people who paid for the privilege, so to speak.

I am going to take full advantage of the situation by going over some ancient history of the safety Rensselaer Polytechnic Institute research program, telling how some things began, drawing some conclusions, and even giving some recommendations. That is what I have learned to do as a member of the Defense Nuclear Facilities Safety Board; we exist to make recommendations to the Secretary of Energy. And incidentally, if the first person singular is used a lot in what follows, that's mostly because I am trying to tell of things in which I had some part and so can speak with authority.

Let me just state at the outset that this meeting is, I believe, the twenty-six in a series that I began in 1973. I'll say a little more about that later.

We start the story in the middle 1960s, a little more than thirty years ago. I was Chairman of the Advisory Committee on Reactor Safeguards (ACRS) at the time. The initial flood of orders for new nuclear plants was just beginning; designs were quite mobile. The Regulatory Staff of the Atomic Energy Commission (AEC), later to become the Nuclear Regulatory Commission, was quite small. A few of the staff members came to a meeting of the ACRS and told us that some scoping calculations made by theorists at the National Reactor Testing Facility at Idaho (as it was then called) indicated that if a reactor completely lost its supply of cooling water the temperature of the fuel would continue to rise until the core melted, and then it would melt through the vessel and fall on the floor of the containment building, and it would keep on going. Thus was born the "China Syndrome." I left ACRS a little later, but stayed in touch.

The next important step in the sequence occurred when a Committee was appointed by Harold Price, who was then Director of Regulation for the AEC, to investigate the reality of the scoping calculations. This was a group headed by William Ergen of Oak Ridge. The Ergen Report confirmed the reality of the threat, and strongly stressed the absolute importance of prevention of loss of coolant through what are now called "engineered safety features," which reactor designers had already begun to include in their designs. Incidentally, the fact that the designers were proposing these features on their own, with no prior urging, has convinced me later that the astute theorists at commercial reactor designer companies had already reached the conclusions on their own.

The Ergen Report led the Reactor Development Division of AEC to initiate several programs at the Idaho Facility, to test performance of Emergency Core Cooling Systems (ECCS) for Pressurized Water Reactors (PWRs). Loop sized experiments called "semiscale" were begun, to be followed by the LOFT experiment, where a small PWR was to be subjected to loss of coolant along with function of a scaled emergency core cooling system. Programs for testing emergency core cooling of Boiler Water Reactors were run by industrial groups at the Moss Landing Facility of the Pacific Gas and Electric Company. Some related experiments were run with electrically heated bundles of simulated fuel elements at Oak Ridge and Westinghouse; the last set were jointly funded by AEC and Westinghouse, and they explored effects that might result from damage to fuel cladding at the elevated temperatures and reduced pressures of a loss of coolant accident. All of these operations were in accordance with a program plan formulated by a group at the Idaho facility.

At the time, the primary attention of the Reactor Development Division was focussed on development of the Fast Neutron Breeder concept, and the design of the Fast Flux Test Facility being built at Hanford. A prevalent view was that if nuclear plants were built and operated according to strictly enforced standards, there would be no loss of coolant accidents, or any other large accidents.

A number of the scientists engaged in the safety research programs chafed under what they perceived as inadequate attention to research programs to determine effectiveness of systems designed to mitigate the accident if it were to start. The unrest reached the ears of Ralph Nader, who then instituted a suit to require shutdown of all operating nuclear reactors, on the grounds that their safety was not ensured. To address the question, the Atomic Energy Commission called a public hearing to explore the question. The courts deferred consideration of shutdown of the reactors pending outcome of the hearings.

As is customary, regulatory hearings are of the judicial form. That is, intervenors act like prosecutors, and they can call their own witnesses and can cross-examine other witnesses. They did so with a vengeance in the ECCS hearings (as they were called). There were about 26,000 pages to the hearing record. I know, because I had to read every one.

A number of researchers in the programs testified, many of them expressing views that information underlying effectiveness of the ECCSs was not adequately reliable or even that it showed the analytical tools for designing the systems were wrong. Early on, the five members of the Atomic Energy Commission headed by Jim Schlesinger realized that they were not going to be able to deal with a judgement on the results of the hearing. They asked two people, Herbert McPherson of Oak Ridge and the University of Tennessee, and me, to follow the hearings and to propose a response for the Commission to make.

The two of us after long and hard work drafted a report which the Commission accepted and issued verbatim as their opinion. The central feature of that opinion was a set of requirements on computer codes that AEC would permit being used to justify effectiveness of Emergency Core Cooling Systems described in license applications. The Regulatory Staff converted these to the Appendix K to 10CFR50.

Appendix K became notorious after a time, because it was so prescriptive on acceptable features of computer codes used to design ECCSs, and contained such conservatism. Unfortunately, all of that was necessary at the time, because the prescribed technology had to circumscribe features of the technical understanding of phenomena as they were brought out by the hearing.

The opinion also promised a safety research program to firm up the basis for acceptable features of the computer codes, and to permit relaxation of the requirements where that became possible. The courts concluded that the

Commission's opinion satisfied requirements for the time being, and noted that the promise of the safety research program offered to solve the problem in the long term. Conduct of the safety research program came to be called "paying off the mortgage on the power reactor program." The mortgage was to be considered paid off when the ECCS computer codes were regarded as reliable, and when they predicted acceptable behavior of the systems.

By this time Schlesinger had left the Commission and Dixie Lee Ray had become the Chairman. She drafted me to head the research program as Director of a new Division of Reactor Safety Research. After an ineffective struggle to escape I agreed to do so. With the argument that the Regulatory Staff needed to have an independent basis for deciding the validity of the technical propositions it had to consider in reactor licensing, I managed to obtain resources needed for a rapidly growing program of "confirmatory research." Though the central feature of that program was development of new computer codes for predicting response of reactor systems to ECCS, development of input data needed for the codes, and testing of prediction capability in experiments up to and including operations with the LOFT facility, other components were added, including such topics as structural reliability of piping and vessels, and safety of fast breeders and High Temperature Gas-cooled Reactors. I would be remiss if I did not mention the singularly important contributions by Dr. Long Sun Tong in achieving the goals of the research on water reactor safety.

I left the program in 1976, a year after it had been transferred to the new Nuclear Regulatory Commission. It continued to be enlarged under Saul Levine and Bob Budnitz, and the mortgage was finally paid off by the series of LOFT tests, where ECCS performance was conservatively predicted by safety codes which had been developed at Los Alamos and Idaho. I won't go into details here because many of you participated in these phases of the program, and I was off doing other things.

The important thing to note is that the nuclear power plants operating today owe their continued existence to the safety research program that is represented here. You developed an entirely new branch of engineering: that of nuclear power plant safety.

Now I'll turn to another part of nuclear plant safety in which I've been a fringe player since its beginning. This is risk assessment.

In 1956 the first commercial power reactors were about to go on line. Congress struggled with legislation to protect the fledgling industry from any financial cataclysm from accidents to nuclear power plants. The Commission asked Brookhaven National Laboratory to conduct a study to estimate the consequences of such an accident. A group was formed within my Division at Brookhaven to attempt this. The result, published as a report numbered WASH-740, was not very helpful, because it concluded that if the containment worked, there would be no damage to surrounding population, and if containment failed, only the upper bound of consequences could be estimated, from liberation of all fission products in the form of noble gases, a large fraction of the radioiodine, and some fraction of the other fission products. The public damage from that would be enormous. In a rare example of common-sense legislation, Congress issued what became known as the

Price-Anderson Act to provide the protection needed by the industry, and in doing so it ignored the upper limit estimates of WASH-740. That Act established a fund containing contributions by nuclear utilities of a portion of their revenues from nuclear electricity. The fund was for coverage of expenses following a conceptual accident, and for public compensation in that event. It was enough for the industry to go ahead with development of the field.

In 1966 the Act had to be renewed, and a second study at Brookhaven for this purpose led to a conclusion that by and large the earlier results could not be improved on. Some years later, as the time approached for a second consideration of renewal of the Act, Harold Price called me to ask if I personally would head a new study, also to estimate probabilities of accidents. I said I did not think that could be done, but suggested Norman Rasmussen of MIT as one who could try. Well, you all know the results; Norm with the help of Saul Levine and other contributors did an incredible job. He succeeded in accomplishing the impossible, and WASH-1400 was born.

Dixie Lee Ray also asked me to fold management of Rasmussen's project into my new Division of Reactor Safety Research, which was easy since Saul Levine was already my deputy. Before the Report was issued, I read every word of it and its voluminous appendices, and I did much of the technical editing on it. After I left the safety research program, I continued active in numerous meetings and discussions on WASH-1400 and the successor program that led to NUREG-1150.

This is all by way of my leading up to some remarks on the uses of risk assessment. There is a lot of discussion these days directed to risk-based regulation. I must say that there is more danger of over-use of this concept than there is to be attached to its under-use.

Levine and Rasmussen were always firm in their statements that the large error bars should be the basis for avoiding use of bottom line estimates of risk. Risk estimates should be used primarily as a basis for regulation that remains solidly founded on mechanistic requirements, with emphasis on <u>a basis</u> rather than <u>the basis</u>. I thoroughly agree. Risk analysis can be very powerful in a number of ways. It can be used to identify vulnerabilities in design and operation of plants by searching for major contributors to accident probability and consequences. It can be used as an aid to choice among alternatives in design or operation because many contributors to error bars cancel out in comparisons of risk. But where risk analysis is used in such ways, the conclusions should always be subjected to reality checks. The question should be asked: does this result make sense? If not, what is the source of the problem? It is not only important that regulators recognize such points; it is important that they continue to pass the information on to the less-technically-prepared groups that often try to push use of risk methods too far. I read that there are now pressures from some parts of Congress to do more risk-based regulation. What do they mean?

Some final remarks. The first of these meetings of the reactor safety research community in 1973, was attended by only a sparse number of researchers from a few laboratories. This was just after the trauma of the ECCS hearings, and attendees were afraid to talk about their research. When I asked for people to speak, I got only silence.

I had to harangue the group and tell them that I not only had to hear what they were doing but I insisted that they had better start publishing the results in the open literature or there would be hell to pay. A few people then began to talk about their work, and a trickle of publications began to appear in subsequent months, that later swelled to a torrent. Well, this meeting like so many of its predecessors shows that the problem of reluctance in 1973 no longer exists. Hallelujah!

Appendix C: Reviews for the Journal of Fluid Mechanics Manuscript "One-Dimensional Two-Phase Flow Equations and Their Characteristics"

These reviews were typed and not prepared using word processors since they did not yet exist. Therefore I followed their formatting as closely as possible.

Reviewer A
Referee's Report on "One-Dimensional Two-Phase Flow Equations and Their Characteristics" by D. Gidaspow, R. W. Lyczkowski, C. W. Solbrig and E. D. Hughes

General Comments

This reviewer is unable to find in this paper a rational physical concept justifying the equations for one-dimensional two-phase flow proposed by the authors. The only justification offered appears to be the condition that their system leads to well posed initial value problems for finite volume fractions, while presently proposed equations do not. A stronger condition, either physical or mathematical, should be given if the paper is to warrant publication.

Detailed Comments

1. Averaging process used in their equations is not defined explicitly.
2. No explanation given for the neglection (sic) of the diffusive, energy, or virtual mass terms in their suggested equations.
3. It is not proved explicitly that Eq. (3) is valid when a change of phase takes place in the flow.
4. The set of equations the authors are trying to prove wrong (according to the authors) lead to a well posed initial value problem when the velocities of each phase are equal but not when they are unequal. The reviewer suspects that diffusive or virtual mass type terms may be important and they lead to the change in the mathematical character of the equations. It is not evident as stated earlier that the changes suggested by the authors are physically justified.

Reviewer B
Referee's Report on:

"One-dimensional two-phase flow equations and their characteristics".

By:

D. Gidaspow et al.

R.W. Lyczkowski, *The History of Multiphase Science and Computational Fluid Dynamics*, Mechanical Engineering Series,
https://doi.org/10.1007/978-3-319-66502-3

Writing on two phase flows without specifying the topology is a hazardous enterprise, as this paper illustrates. When one does not consider a specific type of two phase flow, as for example fluid droplets in air or gas bubbles in liquid, one cannot make an, even approximate, concept about the transfer of mass, momentum and energy between the phases. In simple configurations this is already a difficult task.

We are still far from description of these transfer mechanisms for general two phase flows. So, it is no surprise that, when still trying to give such a description, one finds no conclusive arguments to solve controversial points as the one discussed in the present paper: the question whether in the momentum equation for the single phases one would write

$\partial(\alpha P)/\partial x$ or $\alpha \partial P/\partial x$

The authors try to solve this problem by, what seems to me, a very indirect method, which runs as follows: Write down the equations for conservation of mass, momentum and energy, and the constitutive laws, and find the characteristics of the motion. That formulation of the pressure gradient term (see above) which leads to real characteristics, is the appropriate one, because "equations with complex characteristics lead to ill posed initial value problems".

My first objection is that there are no reasons to expect a totally hyperbolic system of equations in practical circumstances. There is no proof or evidence that for a general liquid-gas flow the system of equations should be totally hyperbolic.

So, the test applied by the authors is in no way decisive for the assumed equations.

A second objection concerns the notion of characteristics as used by the authors (in the case in which, as they assume, the equations are quasi linear with no derivatives in the "right hand side").

They state that characteristics have thus far not been used in two phase flow. I don't know whether this is true or not but anyway, this may have its reasons.

In nonequilibrium flows as the authors are dealing with, the characteristics have no longer the meaning which they have in classical gasdynamics. There the characteristics give the paths along which the Riemann invariants propagate unchanged. Here signals are dispersed and attenuated as they propagate. The best way to find the speed with which disturbances propagate is to linearize the equations and to insert solutions of the form exp i(kx - ωt). Examples from two phase flows of this technique are in F.K. Marble's review (Ann. Rev. Fl. Mech. 2, 1970) on dusty gases and van Wijngaarden's review, mentioned in the paper, on bubbly flows. The use of characteristics asks special caution, as is well understood by know in nonequilibrium gas dynamics. See, for example: Nonequilibrium Flows edited by P. Wegener, Marcel Dekker Inc. New York, 1970. From this field we know that in case of nonequilibrium and finite transfer rates the characteristics give, apart from the particle speeds, the lines $dx/dt = u + c_f$, where c_f is the "frozen sound speed", defined by

$$c_f^2 = -\frac{\rho(dH/dP)}{\rho(dH/dP) - 1}$$

where H is the enthalpy per unit mass.

In a search for the dispersion equation of small amplitude waves, one finds c_f as the speed with which disturbances of infinite frequency propagate. The authors do not obtain the quantity c_f from their calculations. I suspect that the reason for this is that they assumed the pressures in both phases to be equal, (but the velocities and temperatures not). In that case the set of equations do not have the properties of characteristic equations, (see for a similar case the article by L.J.F. Broer in the mentioned book edited by P. Wegener). The proper way to handle this, would-be to prescribe the relations for transfer of heat and momentum and to leave the pressures as they are. (The point is that as a result e.g. of heat transfer the variable parts of the pressures and densities are not in phase if a wave passes and one cannot therefore prescribe that the pressures are equal).

When the rates of transfer are infinitely large there is equilibrium. Temperature, velocity and pressure are equal in that case for both phases. Also in that case the method of characteristics gives meaningful results. One finds $dx/dt = u + c_e$, when c_e is the "equilibrium speed" which for a liquid gas mixture takes the value c_m as defined in the paper. In the appendix to the paper the authors find c_m indeed by the method of characteristics, but this result is rather obvious and does not warrant an appendix.

Summarizing this comment: The applied test is not conclusive for the problem of the proper form of the pressure gradient term. The set of equations is debatable as a starting point for the method of characteristics. The results can be trusted only for the case of complete equilibrium, but then the result is almost trivial.

(Note: The poor English and grammar above are exactly as in the reviewer's manuscript. RWL)

Reviewer C

Referee's Report on

"One-Dimensional Two-Phase Flow Equations and Their Characteristics"

by D. Gidaspow, R. W; Lyczkowski, C. W. Solbrig and E. D. Hughes

This paper examines two phase flow equations with slightly different forms and finds their characteristics. The major concern is whether the volume fraction α is inside or outside of the derivative of the pressure force in the momentum equation. An additional section concerns the characteristics when an "added mass" term is in the equation.

The authors have a preconception that the flow should be solved as an initial value problem and have real characteristics. The major emphasis on their results is the mathematical nature of the characteristics.

What is lacking in this paper is discussion of the physics behind the equations and the physical interpretation of the results. The authors make no physical judgments as to whether the proper pressure force term has α inside or outside the differential. It is improper to imply that equations which result in well posed initial value problems are correct. Unsteady incompressible flow of a single phase doesn't have real characteristics to my knowledge.

Likewise in their discussion of the "added mass because of acceleration" there is no physical discussion of the origin of the term nor its results. The added mass of a body in an incompressible potential flow is the result of extra pressures on the body surface. These pressures are required to accelerate the continuous fluid and change the flow field to that appropriate to the new body velocity. These pressure propagate essentially instantaneously through the fluid in incompressible flow. It would seem that the elliptic nature of these terms might be entirely reasonable. The authors imply that an ad hoc expression involving $\partial/\partial t$ is superior because it gives real characteristics while d/dt does not. I would appreciate arguments which were put on a physical basis. Another point: In situations where particle or bubble acceleration is important the added mass concept deemphasizes the fact that extra pressure forces between the phases are actually at work. This may invalidate the assumption that the average pressure gradients of the phases are equal.

On the same subject of the assumed pressure equality between bubbles and liquid, I would like to mention the acceleration effects in a liquid caused by bubble size changes. This effect is the radial analogy to the added mass effect in linear momentum changes. The basic problem for growth or collapse of a bubble in an incompressible fluid is given in several texts. The only person to employ this effect in the two phase equations that I know of was a Cal Tech student.

In summary, the authors have done some interesting calculations but I would not recommend publication without a thorough discussion of the physical aspects of these equations and interpretation of the results.

Reviewer D

Referee's Report on

One-Dimensional Two-Phase Flow Equations and Their Characteristics

by D. Gidaspow, et al.

I recommend against publication of the subject paper for the following reasons:

1.) The proposed formulation assumes implicitly that the two-phase mixture is homogeneous over distances small in comparison with the physical lengths of the problem. For problems of moderate or high condensed volume fractions this is not true. The formulation is valid over a quite restricted range of volume fractions.
2.) The paper cites a mathematical difficulty arising from a certain model of the continuum problem. This implies that the physics of the model or the problem is incorrect. This situation calls for serious work on the construction of the physical model, not an exhaustive exhibition of the values of physical parameters that lead to complex characteristics.
3.) The physical penetration which the paper makes is minimal and misleading. It consists in some doubt as to how the "pressure gradient" terms appear and a conjecture about transient inter-phase forces. There is no doubt about the description of each phase as a continuous medium and the detailed continuum-like equations for the two-phase motion involve local integration over the phase boundaries and averaging over a region small with respect to problem

geometry. There are circumstances where this process may break down. It may be the tendency of the fluid to form into single phase fluid masses that are of the same order as the -geometric length. There may, in fact, be some question in this case about a physically correct initial value problem.

4.) In short, the results of the authors' numerical calculations demonstrate that they were made using an inadequate physical model. The resolution of the inadequacies and formulation of a simple but physically satisfactory model for the heavily-loaded initial value problem would be interesting and worthy of publication. But this is not carried out in the subject manuscript.

Appendix D: Extracts from reviews of the manuscript "Characteristics and Stability Analysis of Transient One-Dimensional Two-Phase Equations and Their Finite Difference Approximations" by D. Gidaspow, R.W. Lyczkowski, C.W. Solbrig and E.D. Hughes for the session Fundamentals of Two-Phase Flow at the 1975 Winter Annual ASME Meeting, Houston, Nov. 30-Dec. 4, 1975

Reviewer I. This review amounted to a total of one and a half single spaced pages The most relevant comment was "The authors discuss the position of the void fraction in the pressure gradient as if it were arbitrary, and could be put where one liked to insure a hyperbolic system. Clearly this is nonsense. In fact it is well known that equation (2) in their paper is incorrect." **My response**: "I can only refer to such two-phase flow experts as Soo and Pai who believe in the existence of a partial pressure. Einstein in his book 'Investigations on the Theory of the Brownian Movement' on pages 9 and 10 derived a momentum balance by minimizing the energy of the system. He derived a diffusion form which can be interpreted in terms of a partial pressure." Dimitri contributed to this response.

Reviewer II. This review amounted to two and a half pages had basically the same concerns as **Reviewer I** and is discussed by me above. The bulk of the review concerned itself mostly typographical and grammatical items.

Reviewer III. This review amounted to a total of one and a half pages. It was the only one recommending rejection. Referring to the issue of the void fraction being inside or outside the pressure gradient, the reviewer stated "In fact, it depends on what enters the interaction terms! If the void fraction is outside, the interaction term involves only the friction drag whereas if the void fraction is inside, the interaction term involves the total drag (buoyancy + drags)." The bulk of the review concerns mostly typographical and grammatical items. **My response**: The comment is somewhat irrelevant. The more important point is deciding if the drag terms are expressible as differential or not."

Reviewer IV was extremely short and had the issue with the form of the pressure gradient term.

Reviewer V. This reviewer was quite constructive and stated "The problem of a central theme is…critical…". My response: The problem of a central theme has hopefully been cleared up by a stronger abstract. We desired to study the

R.W. Lyczkowski, *The History of Multiphase Science and Computational Fluid Dynamics*, Mechanical Engineering Series,
https://doi.org/10.1007/978-3-319-66502-3

mathematical nature of the equations and not get too much into the physics in this paper." Once again the bulk of the review concerned itself mostly typographical and grammatical items.

Appendix E: Discussion on the ASME paper 75-WA/HT-25 “Characteristics and Stability Analysis of Transient One-Dimensional Two-Phase Equations and Their Finite Difference Approximations” by D. Gidaspow, R.W. Lyczkowski, C.W. Solbrig and E.D. Hughes for the session Fundamentals of Two-Phase Flow at the 1975 Winter Annual ASME Meeting, Houston, Nov. 30-Dec. 4, 1975

R.W. Lyczkowski, *The History of Multiphase Science and Computational Fluid Dynamics*, Mechanical Engineering Series,
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DISCUSSION ON ASME PAPER 75-WA/HT-23

Characteristics and Stability Analyses of Transient One-Dimensional Two-Phase Flow Equations and Their Finite Difference Approximations*

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DISCUSSION PREPARED BY:

1. J.A. BOURÉ, J.M. DELHAYE, AND A.J. LATROBE, SERVICE DES TRANSFERTS THERMIQUES, CENTRE D'ETUDES NUCLÉAIRES DE GRENOBLE, FRANCE

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REPLY PREPARED BY THE AUTHORS.

THIS DISCUSSION PREPARED ON BEHALF OF THE AMERICAN SOCIETY OF MECHANICAL ENGINEERS, HEAT TRANSFER DIVISION, FOR THE 1975 WINTER ANNUAL MEETING, HOUSTON, TEXAS, FOR THE SESSION ON FUNDAMENTALS OF TWO-PHASE FLOW.

Comments on a paper entitled "Characteristics and Stability Analyses of Transient One Dimensional Two-Phase Flow Equations and Their Finite Difference Approximations "by R.W. LYCZKOWSKI et al.

Comments by J.A. BOURÉ*, J.M. DELHAYE* and A.J. LATROBE*

The above paper would certainly justify several comments. A general comment may first be made on the necessity of close interactions between the physical, mathematical and numerical points of view to achieve progresses in the field.

However, the comments made hereunder are limited to three specific topics, which are of fundamental importance in two-phase flow modeling problems, namely :

- mathematical nature of the set of equations (i.e. hyperbolic or not)
- form of the pressure gradient term in the momentum equation (i.e. $\frac{\partial(\alpha P)}{\partial x}$ or $\alpha \frac{\partial P}{\partial x}$. Incidentally, a similar problem may be encountered in the energy equation, with $\partial/\partial t$ derivatives)
- soundness of the procedure consisting in the replacement of some equations (such as the energy equations) by assumptions on some dependent variables (such as the temperatures).

1. Mathematical nature of the set of equations

1.1 - It must be pointed out first that, in practice, a two-phase flow problem cannot be regarded as a pure initial value problem. Boundary conditions are necessarily involved, at least near the inlet of the system, and in most cases (i.e. when the flow is not choked) near the outlet. However, the initial value approach used by the authors is valid locally for most computational meshes.

1.2 - Although it may be argued that, very often, the results obtained with linearized equations are valid for non-linear equations, it must be recalled that the theorems used by the authors to demonstrate the necessity of real characteristics are valid only for partial differential equations with variable coefficients, whereas the two phase flow equations are completely non-linear. Hence the obtained results, if plausible, have no absolute value.

1.3 - The standard Von Neumann stability analysis applies to sets of equations which have only real characteristics. Therefore, the interpretation of complex characteristics, as given by the authors (namely that disturbances grow exponentially for all wavelengths if complex characteristics are present) is not valid. In their section 6 the authors only show that, if the solutions have the form $u(x, t) = f(x) g(t)$ - a very particular form - they are not bounded when complex characteristics are present.

1.4 - In their section 7, the authors enlarge the region where the characteristics are real by putting some derivative of a dependent variable $\partial\alpha/\partial x$ in the momentum transfer term. Although such a trial and error method cannot be used to justify the presence of derivatives in the transfer terms, it may be of interest to notice here that the necessity of such terms can be demonstrated (2).

2. Form of the pressure gradient term in the momentum equation.

The instantaneous area-averaged equations are obtained by means of the following limiting forms of the Leibniz and Gauss theorems (1) :

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1 - Limiting form of the Leibniz theorem :

$$\frac{\partial}{\partial t}\int_{a_k(z,t)} f(x,y,z,t)\,da = \int_{a_k(z,t)} \frac{\partial f}{\partial t}\,da + \oint_{\mathcal{C}(z,t)} f\,\mathbf{v}_{a_i}\cdot\mathbf{n}_k \frac{d\mathcal{C}}{\mathbf{n}_k\cdot\mathbf{n}_{k\mathcal{C}}} \quad (1)$$

$a_k(z,t)$: cross section area occupied by phase k

$\mathcal{C}(z,t)$: intersection line between the interface A_i and the reference cross-section plane

$\mathbf{n}_k$: unit vector normal to A_i, directed outward phase-k

$\mathbf{n}_{k\mathcal{C}}$: unit vector normal to $\mathcal{C}$, located in the reference cross-section plane and directed outward phase k.

$\mathbf{v}_{a_i}\cdot\mathbf{n}_k$: speed of displacement of A_i

2 - Limiting form of the Gauss theorems :

$$\int_{a_k(z,t)} \nabla\cdot\mathbf{B}\,da = \frac{\partial}{\partial z}\int_{a_k(z,t)} B_z\,da + \oint_{\mathcal{C}(z,t)} \mathbf{n}_k\cdot\mathbf{B}\,\frac{d\mathcal{C}}{\mathbf{n}_k\cdot\mathbf{n}_{k\mathcal{C}}} \quad (2)$$

$$\int_{a_k(z,t)} \nabla\cdot\overline{\overline{T}}\,da = \frac{\partial}{\partial z}\int_{a_k(z,t)} \mathbf{n}_z\cdot\overline{\overline{T}}\,da + \oint_{\mathcal{C}(z,t)} \mathbf{n}_k\cdot\overline{\overline{T}}\,\frac{d\mathcal{C}}{\mathbf{n}_k\cdot\mathbf{n}_{k\mathcal{C}}} \quad (3)$$

$\mathbf{n}_z$: unit vector normal to the reference cross-section plane

Particular case :

$$\mathbf{B} = \mathbf{n}_z$$

$$\frac{\partial}{\partial z} a_k(z,t) = -\int_{\mathcal{C}(z,t)} \mathbf{n}_k\cdot\mathbf{n}_z \frac{d\mathcal{C}}{\mathbf{n}_k\cdot\mathbf{n}_{k\mathcal{C}}} \quad (4)$$

Starting from the local instantaneous momentum equation written for phase k, we obtain for the area-averaged equation projected along the axis of the channel :

$$\begin{aligned}
&\frac{\partial}{\partial t} a_k\langle\rho_k w_k\rangle + \frac{\partial}{\partial z} a_k\langle\rho_k w_k^2\rangle - a_k\langle\rho_k F_z\rangle \\
&+ \frac{\partial}{\partial z} a_k\langle p_k\rangle - \frac{\partial}{\partial z} a_k\langle(\mathbf{n}_z\cdot\overline{\overline{\tau}}_k)\cdot\mathbf{n}_z\rangle \\
&= -\int_{\mathcal{C}(z,t)} \mathbf{n}_z\cdot(\dot{m}_k\mathbf{v}_k - \mathbf{n}_k\cdot\overline{\overline{T}}_k)\frac{d\mathcal{C}}{\mathbf{n}_k\cdot\mathbf{n}_{k\mathcal{C}}} \qquad (5) \\
&+ \int_{\mathcal{C}_k(z,t)} \mathbf{n}_z\cdot(\mathbf{n}_k\cdot\overline{\overline{T}}_k)\,\frac{d\mathcal{C}}{\mathbf{n}_k\cdot\mathbf{n}_{k\mathcal{C}}}
\end{aligned}$$

with : $<f_k> \triangleq \frac{1}{A_k(z,t)} \int f_k(x,y,z,t)\, dA$

ρ_k : density
w_k : z – component of the velocity vector
F_z : body force per unit of mass
p_k : pressure
τ_k : viscous stress tensor
$\mathbb{T}_k$: total stress tensor
$\dot{m}_k \triangleq \rho_k(v_k - v_i)\cdot n_k$: mass flux at the interface

(relative to phase k)

$\mathscr{C}_k(z,t)$: wall perimeter in contact with phase k.

Important remarks Eq. (5) :

1. The only hypotheses necessary to derive Eq. (5) are :
   a. the wall is motionless
   b. there is neither injection nor succion through the wall
2. A_k is inside the $\frac{\partial}{\partial z}$ in the pressure term
   but
3. the total stress tensor $\mathbb{T}_k$ enters the line integrals $\int_{\mathscr{C}}$ and $\int_{\mathscr{C}_{ik}}$

Let us assume now that the pressure p_k is constant over A_k (z,t) at time t, that is :

p_k is a function of z and t only

so that $<p_k> \equiv p_k\,(z,t)$ (6)

By using Eq. (4) and by recalling that :

$$\mathbb{T}_k = -p_k \mathbb{U} + \tau_k \qquad (7)$$

we obtain from Eq. (5) :

$$\begin{aligned}
&\frac{\partial}{\partial t} A_k <\rho_k w_k> + \frac{\partial}{\partial z} A_k <\rho_k w_k^2> - A_k <\rho_k F_z> \\
&+ A_k \frac{\partial p_k}{\partial z} - \frac{\partial}{\partial z} A_k <(n_z \cdot \tau_k)\cdot n_z> \\
&= -\int_{\mathscr{C}(z,t)} n_z \cdot (\dot{m}_k v_k - n_k \cdot \tau_k)\, \frac{d\mathscr{C}}{n_k \cdot n_{k\mathscr{C}}} \qquad (8) \\
&+ \int_{\mathscr{C}_k(z,t)} -n_z \cdot (n_k \cdot \tau_k)\, \frac{d\mathscr{C}}{n_k \cdot n_{k\mathscr{C}}}
\end{aligned}$$

Important remarks concerning Eq. (8)

1. A_k is outside the $\frac{\partial}{\partial z}$ in the pressure term
   but
2. the viscous stress tensor τ enters thé line integrals $\int_{\mathscr{C}}$ and $\int_{\mathscr{C}_k}$
3. the only supplementary hypothesis is Eq. (6)

It can be concluded that both forms (5 or 8) are acceptable, provided the other terms are properly written.

3. Soundness of the procedure consisting in the replacement of the energy equations by assumptions on the temperatures.

Although the authors only suggest the possibility of such a procedure (in their section 2), its very current use in the two-phase flow literature and its drawback justify a discussion :

In single phase flow models, the nature of the evolution of the fluid (e.g. isentropic, isothermal ...) is often specified a priori. A more general and rational procedure, however, is to postulate the transfer laws (cause) rather than the nature of the evolution (effect). This procedure yields models which include as particular cases all the conceivable evolutions.

For one-dimensional single phase flows, the nature of the evolution is often known in practice, since all the transfers take place at the wall. Such is not the case for two-phase flows, for which no simple assumptions can be made on the thermodynamic evolutions of the phases because of the importance of the interfacial transfer processes (mass, momentum, energy). Specifying the evolution of some variables implies strong constraints on the transfer terms (even if numerically the actual and postulated evolutions are close to each other).

For instance if, as often assumed, the gas-phase remains at saturation, the interfacial heat transfer must exactly compensate for the variations of T_{sat} due to pressure drops.

The above constraints may be shown (3) to have major non-physical consequences, such as the impossibility for the corresponding flow to reach choking. Therefore, the replacement of equations by assumptions must be avoided whenever possible.

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Comments on a Paper Entitled "Characteristics and Stability Analyses of Transient One Dimensional Two-Phase Flow Equations and Their Finite Difference Approximations" by R. W. Lyczkowski et al.

Comments by M. Ishii
Reactor Analysis and Safety Division
Argonne National Laboratory

The paper discusses interesting numerical instability problems associated with the two-fluid model formulation and numerical schemes based on the hyperbolicity of the system. I have three specific comments.

I) Pressure Gradient Term (p. 2, 2nd paragraph; p. 2∼7)

The authors studied and compared the numerical stability of the systems having

i) $\alpha^{a} \frac{\partial p}{\partial x}$

or

ii) $\frac{\partial(\alpha^{a} p)}{\partial x}$

as the pressure term in the momentum equation. The first form is commonly used in two-phase flow analyses and it can be easily justified on a physical base, whereas the second form has little basis for two-phase flow systems with interfaces. This point is explained below.

The rigorous averaging applied to a local instant formulation (Delhaye (6), for example) as well as a simple control volume analysis can show that the pressure term should be (see Fig. 1)

$$\frac{\partial(\alpha^{a} p)}{\partial x} - p_i \frac{\partial \alpha^{a}}{\partial x}$$

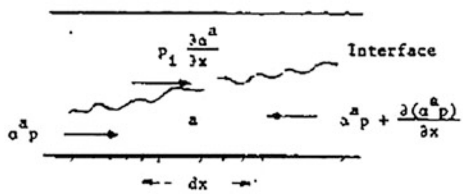

Fig. 1

where p_i is the pressure at the interface. If we can assume that $p_i = p$, then the pressure term reduces to $\alpha^a \frac{\partial p}{\partial x}$. The second term in the above expression is the pressure force acting at the interface in the direction of main flow and it may not be neglected. Therefore, the authors' stability analysis for the system with only $\frac{\partial(\alpha^a p)}{\partial x}$ term appears less interesting. Actually, omitting of a term associated with an interface is a common mistake as I quote from a standard text book by S. Whitaker (Introduction to Fluid Mechanics, Prentice-Hall, 1968, page 237, last paragraph, in a discussion on a macroscopic force balance)

> "..... experience has shown that students will often neglect this term. The reason appears to be associated with a general error made in the analysis of macroscopic balance problems - i.e., focusing attention on entrances and exits and completely forgetting about other surfaces." (end of quote)

II) Hyperbolicity and Numerical Instabilities

It is not surprising to find that the system (with $\alpha^a \frac{\partial p}{\partial x}$ in the momentum equation) is unstable if it is solved as an initial value problem. The instabilities caused by the relative motion between phases for a two-phase flow system with incompressible components is known as the Kelvin-Helmholtz instability. This instability has a physical origin and it can be observed as interfacial waves for a separated two-phase flow system. As discussed by G. B. Wallis in his book (One-dimensional Two-Phase Flow, McGraw-Hill, Chapter 6), the system can be made more stable by introducing sufficiently large differential terms in the interaction terms such as F_x^a. This point has been also discussed in the paper in connection with the transient flow force.

I also like to point out that the introduction of the second order derivative terms associated with the axial diffusions of momentum and energy can have stabilizing effects due to physical dumping of high amplitude waves. Evidently in this case, the equations become second order parabolic.

It should be emphasized here that one should be careful not to eliminate physically important instabilities actually existing in nature (such as flooding, flow reversal, density wave instability, and other well-known two-phase flow instabilities) by introducing artificial terms to preserve the numerical stability.

III) Transient Flow Force Term (p. 5∿7)

The authors have shown that the numerical stability of the system is significantly changed by the introduction of the transient flow force (virtual mass effect) term. It is also interesting to see that the form of the transient flow force term has important effects on the numerical stability. These results indicate the importance of the correct physical modeling of the constitutive equations for the interfacial transfer terms.

The following is a retyped version of our rebuttal sent to Owen Jones retaining as closely as possible the same format.

Rebuttal To Comments on a Paper Entitled "Characteristics and Stability Analysis of Transient One-Dimensional Two-Phase Flow Equations and Their Finite Difference Approximations" by R. W. Lyczkowski et al.

Comments by R. W. Lyczkowski, (1) Dimitri Gidaspow, (2) C. W. Solbrig, (3) and E. D. Hughes (1)

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The authors gratefully acknowledge the written comments of Drs. Ishii, Boure, Delhaye and Latrobe. The comments will be rebutted in the order of highest priority.

I. Drs. Boure, Delhaye and Latrobe

Comment 1.2)
The discussors claim that "very often, the results obtained with linearized equations are valid for non-linear equations, it must be recalled that the theorems used by the authors to demonstrate the necessity of real characteristics are valid only for partial differential equations with variable coefficients, whereas the two phase flow equations are completely non-linear." This statement is false, the two-phase flow equations considered in the paper constitute a system of quasilinear partial differential equations of the first order in two independent variables. (1, 2) The theorems used in the paper are valid for such equation systems. (1, 2)

Comment 1.3)
The first part of this statement is also false. The authors are unaware of any theory of characteristics applicable to partial difference equations. We are also unaware of any restriction regarding the character of the partial differential equations with respect to application of the Von Neumann stability test to the linear finite difference equations. Lax and Richtmyer state concerning the stability of linear difference equations, "Note that we make no reference here to the differential equation whose solution is desired so that stability, as defined, is a property solely of a sequence of difference equation systems." (3)

The authors would appreciate a proof or reference substantiating the first part of the Commentators statement. The authors do agree with Richtmyer and Morton that "if the initial value problem is improperly posed…then no difference scheme that is consistent with the problem can be stable." (4)

Comment 1.1)
We are not analyzing pure initial value problems. This word is never mentioned in the text. We are using the words initial value problem in the sense of Richtmyer and Morton. A quote from page 3 of their text illustrates the usage. "The equations are of such a nature that if a state of the physical system is arbitrarily specified at some

time $t = t_o$, a solution exists for $t \geq t_o$ and is uniquely determined by the equations together with boundary conditions or other auxiliary conditions." (4)

Comment 3)
We thank the commentator for his caveats.

We agree completely that in order for the vapor to remain at saturation, the interfacial heat transfer must exactly compensate for the variations of T_{sat} due to pressure drops.

II. Rebuttal to Common Comments
We thank the commentators very much for their concern over the form of the pressure gradient term. Dr. Ishii is correct by quoting from Whitaker's (5) textbook. He then admits that there are incorrect equation sets in the open literature. Recognized two-phase flow experts such as Professors Soo (6) and Pai (7) believe in the concept of phase partial pressures. Pai goes so far as to say, and I quote "It is interesting to notice [in his Equation (22)] the new interaction term due to the pressure, i.e., $p\nabla z$. z is Pai's nomenclature for solid volume fraction. One is referred to Reference 8 for a transport phenomena control volume derivation of the momentum equations which have the phase volume fractions multiplying the pressure gradient.

III. Dr. Ishii

Comment II)
The similarity between the expressions for the growth rate of the Kelvin-Helmholtz instability and the imaginary part of the complex characteristics of the two-fluid equations was discussed in the Tokyo Round Table Discussion. (9) It should be pointed out that the differential equations which describe the Kelvin-Helmoltz instability have real characteristics.

We point out that we verified the fact that "sufficiently large" differential terms in the interaction terms can stabilize the system as pointed out by Wallis (10) in his Chapter 6.

We recognize that second order differential terms make the system second order parabolic. We only ask, is it necessary to add these terms to resolve the ill-posedness problem?

Comment III)
We thank Dr. Ishii for recognizing what we are trying to point out by analyzing the basic equations with added transient flow forces.

We would mention in passing that Professor Soo recognizes that the ill-posedness of I.V.P.'s for two-phase flow differential equations resulting from complex characteristics may be cured by additional considerations of the interphase forces. (11)

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Appendix F: John Ramshaw's Unpublished Commentary on his Paper with John Trapp

CHARACTERISTICS, STABILITY, AND WELL-POSEDNESS IN TWO-PHASE FLOW

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A contribution to the Forum on Open Questions in Multiphase Flows, 1991 ASME/JSME Fluids Engineering Conference, Portland, OR, June 23–27, 1991.

It is now well known that the simplest and most straightforward description of one-dimensional two-phase flow constitutes an improperly posed initial value problem. This problem has been recognized for over fifteen years, but confusion still persists as to its origin, significance, and proper resolution. It therefore seems worthwhile to revisit the question of why this formulation is ill-posed in the first place and how it should be modified to render it well-posed. Ramshaw and Trapp [1] argued that the problem arises in the improper neglect of short-wavelength phenomena such as viscosity and surface tension, and we continue to believe that this is the essence of the issue. Unfortunately, our discussion has been widely misinterpreted as a mere analysis of surface tension effects. I would therefore like to take this opportunity to restate the essentials of our position as simply as possible.

The concept of ill-posedness is frequently approached via characteristics and mathematical theorems. While characteristics are invaluable for analyzing partial differential equations, they do not provide the clearest approach to ill-posedness. A physically more transparent approach is provided by linearized Fourier stability analysis. In Fourier terms, ill-posedness refers to a situation in which the Fourier growth factor G(k) is unbounded with respect to the wavenumber k, particularly as k approaches infinity (infinitely short wavelength). When this occurs the initial-value problem cannot in practice be solved, because the inevitable short-wavelength

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errors in the initial conditions become arbitrarily large in an arbitrarily short time, thereby destroying the solution. The solution effectively blows up – instantly – in a manner which depends sensitively on the details of the initial errors, no matter how small they are. In contrast, physical instabilities are characterized by finite growth rates for all perturbations. The simplest situation in which this catastrophe occurs is that of separated one-dimensional two-phase flow with unequal phase velocities [1]. The ill-posedness is then due to the fact that this situation is merely a one-dimensional analog of the classical Kelvin-Helmholtz problem, which is known to be ill-posed when viscosity and surface tension are neglected. It is therefore not surprising that the one-dimensional description retains this behavior. Indeed, the analogy is quantitative at long wavelengths, where the one-dimensional two-phase equations predict the same G(k) as a complete two-dimensional analysis [1]. At short wavelengths the one-dimensional description becomes inaccurate and the agreement is only qualitative, but the ill-posedness remains.

To remove this pathological behavior it is merely necessary to restore the physical effects whose neglect gave rise to it. In particular, a simple Fourier analysis shows that either surface tension [1] or viscosity removes the ill-posedness. (Viscosity is actually preferable from a physical point of view, since it is dissipative while surface tension is not. It should also be noted that for numerical purposes it may be necessary to use artificially large values for such parameters, just as one uses an artificial viscosity to treat shock waves. These are sometimes provided by the truncation errors associated with the difference scheme; e.g., the artificial viscosity of donor-cell or upwind differencing). Both of these effects involve higher-order spatial derivatives, and therefore selectively act more strongly on shorter wavelengths. This selectivity is important, as it implies that the effect on longer wavelengths is negligible so that long-wavelength physical instabilities are not removed or otherwise altered. In particular, the Kelvin-Helmholtz instability at finite wavelengths is a real physical instability which the equations can and should properly capture. In contrast, other authors have proposed removing the ill-posedness by introducing ad hoc first-order differential terms that alter the behavior at both short and long wavelengths. Such modifications are both unnecessary and undesirable, as their effects on the long wavelengths are likely to be entirely unphysical. Once the ill-posedness has been properly removed by introducing suitable short- wavelength effects, one may proceed to consider how the physical accuracy of the model may be further improved. This may involve introducing other physical effects (e.g., virtual mass, interfacial inertia, multiphase Reynolds stresses, etc.) as appropriate. Such effects can then be included based solely on their physical importance, and not in the hope that they will magically render the problem well- posed. Some of them may involve first-order differential terms which alter the long-wavelength stability behavior. However, if the formulation is physically correct any such effects on stability will themselves be physical, and the overall fidelity of the model will thereby be improved.

In summary, ill-posed behavior in multiphase flow simply originates in the improper neglect of short-wavelength phenomena such as surface tension and viscosity. Once such effects are included, the formulation becomes well-posed and any further modifications to the model can and should be based solely on the physics of the situation.

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Appendix G: Carl Hocevar's letter of Resignation on September 21, 1974 to Dixie Lee Ray, Chair of the Atomic Energy Commission

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2340 Richards Avenue
Idaho Falls, Idaho 83401
September 21, 1974

Ms. Dixie Lee Ray
USAEC
1717 H Street NW
Washington, D. C. 20545

Dear Ms. Ray:

I am resigning my position as an Associate Scientist with Aerojet Nuclear Company in order to be free to tell the American people the truth about the potentially dangerous condition in the nation's nuclear power plants. As an employee of Aerojet Nuclear I have not been able to freely express my concerns about the nuclear reactor safety issues. Consequently I will be working for the Union of Concerned Scientists in an attempt to more fully inform the public about the current state of knowledge concerning reactor safety, particularly the emergency core cooling systems.

I have been employed at the Idaho National Engineering Laboratory for the past seven years for Aeroject Nuclear and its predecessors. During that time I have been involved in the development of computer codes which are used in the thermnal-hydraulic predictions of loss-of-coolant situations. I was the principal author of the THETA1-B code which was adopted by the AEC as an accepted method of predicting the thermal behavior of a fuel rod during a LOCA. The last several years I have been working on a new thermal-hydraulic loop code. The primary goal of this project is to develop analytical models which will more realistically describe the physical processes that could occur during a LOCA.

While analytical models for predicting the fluid behavior during a LOCA have been developed by both the nuclear industry and the AEC, the techniques in gneral are not capable of describing actual physical situations with a reasonable degree of reliability. The AEC is using shaky and unproven computer predictions as a basis for answering such vital questions as the effectiveness of reactor safety systems in preventing catastrophic accidents. This is wholly unacceptable.

Adequate experimental programs to determine the workability of reactor safety systems are also urgently needed. Experimental verification of the analytical computer codes is a necessity if we are to place our faith in these methods.

Aerojet Nuclear employess were used by the AEC as consultants during the ECCS hearings. In 1971 the AEC adopted the methods we had developed, but completely ignored our reports concerning the serious limitations of those methods. They were the best that could be developed based on the limited analytical and experimental research the AEC and nuclear industry had carried out, but they were preliminary and definitely not an adequately proven way of determining nuclear reactor safety. Little has changed in the past few years, and the safety of nuclear reactors is still uncertain and unverified.

The AEC is ignoring advice from many of its experts on reactor safety problems, a situation that has given rise to numerous resignations. Several of my colleagues have gone to work trying to help the utility companies understand the reactor safety problems that the AEC would prefer to ignore, but I believe that the genral public, and not just the companies investing in nuclear generating equipment, must be told the truth about the potential hazards.

I also have personal reservations concerning the radioactive waste problems. While I am not an expert in waste management I find the long term radioactive waste question deeply disturbing. The present generations get the elctricity from nuclear plants and we leave the radioactive wastes for our children and future generations to take care of. Plutonium, an extremely hazardous material that retains its radioactive potency for hundreads of thousands of years, is hardly a legacy that future generations should be given.

In spite of the soothing reassurances that the AEC gives to an uninformed, mislead public, unresolved questions about nuclear power plant safety are so grave that the US should consider a complete halt to nuclear power plant construction while we see if these serious questions can, somehow, be resolved. The most prudent course of action that we can take is to proceed cautiously.

Sincerely,

Carl J. Hocevar

Cc: Dan Ford, Union of Concerned Scientists

Appendix H: Chemical Process CFD Users Group Charter

PURPOSE: Exploit and enhance the value of CFD in chemical process design for competitive and economic benefit.

OBJECTIVES:

1. Demonstrate the value and feasibility of CFD for process design in the chemical industry.
2. Develop and refine methodologies to take greater advantage of existing CFD tools.
3. Ensure tangible business impact from investment in CFD.
4. Identify new software features that are critical in increasing the economic benefits of CFD and collectively influence software vendors to provide them.

MEMBERSHIP CRITERIA
In order to keep the group at a workable size, encourage exchange of ideas, and keep logistics simple, the following membership criteria are established:

1. Limit to US-based institutions
2. Limit group size to no more than 10 organizations
3. No CFD software vendors
4. Limit of no more than one institution in any of these categories:

Pharmaceuticals	Food
Mixing Equipment	Consumer Products
Computer Hardware	Pulp & Paper
Petrochemicals	Plastics
US Dept. of Energy	Specialty Chemicals
US Dept. of Commerce	Commodity Chemicals
Beverage	

5. Agreement of the entire membership is needed to exceed any of the above limits.

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RESPONSIBILITY OF MEMBERS

1. Each member company has a responsibility to contribute to the CPCFD User Group activities. Such contributions may include one or more of the following:
   a. sharing of experiences with CFD modeling and its importance to the member's organization.
   b. experimental data.
   c. limited person-time to investigate areas of interest to the group.
   d. review and guidance of CPCFD project activities.
2. With respect to intellectual property rights, it should be made clear that all information that is disclosed may be further disclosed. No information is confidential, and it is up to the participants to clear with their own companies what will be said. However, while there is no obligation of confidentiality, no license is granted with respect to disclosed materials, specifically, no patent rights are licensed. Anyone using the information will have to make sure there are no patent rights conflicting with the proposed use.
3. With respect to off-limits topics, the discussions must not deal with competitive information. Discussions of products, product or marketing plans, pricing, sales, etc. should not occur.
4. Each member company will periodically host a CPCFD User Group meeting.

Appendix I: Memorandum of Cooperation for the DOE Virtual Technology Center for Multiphase Dynamics (VCMD)

Purpose

This Memorandum of Cooperation (MOC) recognizes the on-going research collaboration between the US DOE National Laboratories, Facilities, and Energy Centers and (hereinafter referred to as Laboratories), and is set to foster future collaborative research and development ties between these Laboratories. Accordingly, this MOC outlines the general nature of the ties between the Laboratories, identifies activities intended to stimulate and foster collaboration between their researchers. This MOC is intended to provide a basis from which specific agreements and activities will grow and is not intended to limit interactions to those contained herein.

Background

The capabilities at the signatory DOE Laboratories have evolved to represent a significant national resource for development and application toward the DOE missions specifically and toward more general national requirements for Multiphase Dynamics. The Laboratories expertise and facilities are focused upon achieving excellence in solving complex problems using resources across the DOE complex in an effective and collaborative manner.

Stemming from collaborative efforts over the past few years, mutually beneficial relationships between the technical staff at the various Laboratories were recognized. Representatives from these institutions have collaborated on research and development programs in the past and these collaborations have benefited from the combined strengths of the Laboratories and the absence of duplication of effort.

The combining of resources has worked to the benefit of government sponsored research and development in enhancing technical productivity and delivering solutions to our governmental and industrial customers in an effective and efficient manner.

Basis for Agreement

The need to foster basic research, and to transition that basic research to applied research and development is a paramount function of the federal government and it's laboratories. The product of research from the various offices within the Department of Energy needs to be integrated to become more cost effective and

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more widely distributed to both the federal and commercial sectors. One area where the government has and continues to be a clear leader, through it's laboratories, is in the area of multiphase dynamics. The intent of this alliance is to maximize that return on this investment, and to serve as a model for moving other technologies from basic arena to the applied area.

By multiphase dynamics we mean the study of materials in motion in which the motion of one phase relative to another is of major importance, and where the material phases interpenetrate at scales small compared to the overall dimensions of the problem. While this definition is somewhat loose, it provides for a host of problems in which the material motions can be described by separate dynamical equations for each phase coupled by exchange functions for mass, momentum, and energy. Examples include multiphase stirred tank chemical reactors, fluidized beds and bubble columns, some porous media flows, and metal casting. The breadth of applications for multiphase dynamics analysis spans literally from the transport and treatment of municipal waste to the performance of nuclear weapons. Despite the fact that both the Government and the Industrial sectors have a strong perception of value in a computer simulation capability for these widespread applications that is at the same time comprehensive, rigorous and also practical, such a capability has not yet emerged. A consequence of this broad occurrence of multiphase dynamics in modern technology is a correspondingly broad distribution of knowledge on the subject, among scientific disciplines, professional societies, and journal publications. No single organization has emerged as a center of excellence or collector of the knowledge, no comprehensive text has been written, nor is there a movement underway to establish a mechanism for consolidation of the widely dispersed body of information on the subject. The tendency is quite the opposite; the subject is instead continuously subdivided into smaller and smaller subsets leading to a wider and wider dispersion of potentially useful information.

Collaboration among these Laboratories of expertise offers opportunities to perform research beyond the capabilities of the organizations separately. By combining these complementary missions and attributes in a collaborative arrangement, the research teams and the nation attain benefits in increased technical productivity that could not be realized separately. This collection of technology core competency Laboratories cooperating together as a virtual enterprise will allow American industry easy access to the best resources in the nation. Subject to continued Federal and private support in areas of Multiphase Dynamics research and development, it is the intent of this MOC to foster the operation of the DOE Alliance for the Advancement of Multiphase Dynamics (VCMD) to expand the collaboration base now existing. This MOC should provide a basis and stimulus for these interactions to continue and grow.

Special Agreement Elements

Although this MOC is not a binding agreement, it is intended to set forth the understanding among the Laboratories of the preferred processes for carrying out collaborative research and development. The signatories to this MOC will endeavor to accomplish the interactions described below.

VCMD Coordinating Council - A team composed of a representative from each Laboratory will constitute an VCMD Coordinating Council. This council will serve to coordinate and integrate joint activities. These individuals are charged with responsibility for identifying areas of mutual interest, pursuit of joint funding, ongoing research and development collaboration, and other mechanisms including the continued refinement and updating of the VCMD technology roadmap, fostering exchange and enhancement of productivity, reaching the goals defined in the roadmap, and professional development of individual researchers. The council will operate via a permanent chairman/ director.

VCMD Coordinating Council Meetings - Meetings will occur, at a minimum, semiannually or as needed to assure positive and productive collaborative efforts. The chairman will be responsible for calling meetings of the Council.

Program Development - The VCMD Coordinating Council will develop a program development strategy. Each Laboratory will assume a leadership role in developing collaborative research and development programs. Areas, programs, or projects for collaboration will be determined by consensus. Lead responsibilities for a given research area will be determined by consensus. It is agreed that the collaborating Laboratories will have program development activities that are separate from the activities of VCMD.

Collaborative Research Execution - (a) The VCMD Coordinating Council will name a Coordinating Entity for execution, as well as proposed Participating Laboratories, of each project. In turn, the Coordinating Entity will propose to the VCMD Coordinating Council a Principal Investigator who can suggest modification to the proposed group of Participating Laboratories. The VCMD Coordinating Council has final approval authority. (b) Funding for each collaborative project will be divided based on the assigned roles of each of the participating Laboratories. Departures from this arrangement will be by mutual consent of all Coordinating Council members. (c) This MOC shall not be used to obligate or commit funds or as the basis for the transfer of funds. (d) The Coordinating Entity will propose to the VCMD Coordinating Council an Intellectual Property (IP) Coordinator from that Entity who will work with the Participating Laboratories technology transfer offices. The VCMD Coordinating Council has final approval authority of the proposed IP Coordinator.

Roles - The roles of the various Laboratories in any given collaborative research program or project will be determined by updated identification of capabilities and assignment matching research needs and capabilities.

Involvement of Industry - The Laboratories will separately and collectively involve industry in the research and development work. A Multiphase Dynamics technology roadmap will be developed, updated, and validated collectively with industry review panels on an annual basis. The involvement can take several forms including consultation, active solicitation of interfaces with recognized industry associations, identification of areas of industrial interest for cooperative R&D agreements, and direct industrial sponsorship of research and development.

Personnel Exchanges and Visits - In order to encourage collaboration and assist in joint research efforts, personnel exchanges and visits will enable staff to take advantage of opportunities for enrichment and professional advancement. The Laboratories will encourage personnel exchanges and visits wherever mutually beneficial.

Access to Scientific Equipment and Facilities - The Laboratories each have significant and unique research facilities and equipment that are vital to the success of VCMD. Collaborating personnel shall be given access to equipment and facilities, as appropriate, on a non-interfering basis.

Communications Linkages - To facilitate communications as well as contributing to academic programs, the VCMD will investigate the feasibility and appropriateness of the establishment of interactive electronics communication links.

Intellectual Property - Because transferring technology to commercial parties is critical to the success intellectual property rights developed during the performance of work covered by agreements undertaken pursuant to this MOU and to the extent available at the time and to the extent permissible under the DOE Prime Contracts of the individual laboratories, shall be managed in a manner that promotes the best interests of all concerned. Precise terms and conditions will be incorporated into the agreements implementing the specific activities.

Term of This Agreement

This Memorandum of Cooperation shall be in effect for a period of five (5) years from the date of execution thereof and shall remain in effect until that time unless terminated sooner by action of the VCMD Coordinating Council or upon direction by the Department of Energy prior to the scheduled expiration date. Laboratories may remove themselves from this agreement with thirty (30) days written notice to the VCMD Coordinating Council. Then and in either of these events, due consideration will be given to an orderly and timely termination of previous arrangements for personnel exchanges and impacts on program concerns. This Memorandum of Cooperation may be extended upon mutual agreement of the Laboratories.

Appendix J: Review and Comments on the 2006 NETL Technology Roadmap

Review and Comment on the 2006 NETL Technology Roadmap[1]
by Robert W. Lyczkowski, Ph.D., P.E, June 2010

Contents

[1]Work supported by a National Energy Technology Laboratory contract through URS Energy and Construction, Inc. AGREEMENT NO. RES1000062.

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Tables

Figures

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Review and Comment on the 2006 NETL Technology Roadmap

by Robert W. Lyczkowski, Ph.D., P.E.

Abstract
This report is my personal assessment of the 2006 NETL Technology Roadmap, referred to hereafter as simply the Multiphase Roadmap. Included is an historical summary of prior workshop and roadmapping efforts in order to extract lessons learned. The 2006 Report on Workshop on Multiphase Research, referred to hereafter as simply the Multiphase Roadmap report, is reviewed and critiqued. It is concluded that in its present form, it not complete. The organizers and participants did not go through the rigorous procedures established by the DOE employed in the production of its numerous roadmaps. Based upon a review of project reports, workshop presentations, and publications, successes as they relate to the Multiphase Roadmap are presented. Lessons learned from the historical summary form recommendations that should be utilized in improving and completing the Multiphase Roadmap, and to define an effective path forward. A summary of international and national multiphase universities and research laboratories is presented. Due to the shortness of this project, a detailed determination of their multiphase capabilities could not be performed. Two appendices: 1.) summarizing the MED erosion model recommended to be utilized using hydrodynamic outputs from the MFIX computer code, and 2.) a proposal originally prepared for the proposed, but unrealized, DOE Suspension Advanced Research Objective (SARO) which presents a plan for modeling dense liquid-solids flows absent in the Multiphase Roadmap.

1 Introduction

"To know what we do not know is the beginning of wisdom."

Maha Sthavira Sangharakshita

Madhava Syamlal assisted me in organizing two sessions at the AIChE Annual Meeting in Memphis Tennessee on November 11, 2009 titled "Festschrift for Professor Gidaspow's 75th Birthday" to honor our former teacher and Ph.D. thesis advisor at Illinois Institute of Technology (IIT). In Syamlal's presentation "High Resolution Simulations of a Coal Gasifier" [1] he made a quantitative comparison of the Prime computer with present capabilities at NETL. This really tickled me since I mentioned this Prime computer in my paper "The History of Multiphase Computational Fluid Dynamics" [2]. The Prime computer was used in the early 1980's at IIT by students of Professor Gidaspow, starting with Bozorg Ettehadieh, to perform multiphase simulations of fluidized beds.

It was at this venue that Syamlal presented the paper "Roadmapping of Computational Multiphase Flow" [3]. Unaware of what had transpired since the 2006 Workshop on Multiphase Flow Research, I engaged him in a frank discussion concerning my opinions with the precursor of the Multiphase Dynamics Research Consortium (MFDRC) and its proposed predecessor, the DOE Virtual Center for Multiphase Dynamics (VCMD) both supported by the DOE Office of Industrial Technologies (OIT) now the DOE Industrial Technology Program {ITP).

I suggested to Syamlal that I might be able to assist him in his endeavor and he responded by asking what I had in mind. The list of items I proposed were:

1. Define state of the art in multiphase (fluid-solids) modeling, Euler-Euler, Euler-Lagrange, Kinetic theory, vs. DEM, MP-PIC
2. Define experimental needs and measurement techniques.
3. Establish experimental data base-acquisition and management.
4. Provide expert interpretation of phenomena
5. Define additional model validation needs.
6. Define additional research needs w.r.t. multiphase theory, e.g., "turbulence", deterministic chaos, scale-up.
7. Education as to solutions possible via workshops, short courses, hands-on computer laboratory. I gave two courses and one workshop each with Bouilllard and Gidaspow
8. Advisor to commercial CFD software companies needs.
9. Bridge communication breakdown between operating plants and R&D groups.
10. Update National Labs multiphase capabilities.
11. Institute the Hyprotech approach using multiphase CFD (see attached presentation)
12. Assist in implementing the Dean Waters paradigm for a virtual center (presentation attached).
13. Implement the monolayer energy dissipation (MED) erosion model as an add-on to the MFIX code.
14. Determine definitive ROI for CFD modeling.
15. Implementation of the Solutia paradigm for CFD modeling (presentation attached)

Syamlal responded that he was checking around NETL to see what needs to be done to compile a progress report and update the Multiphase Roadmap. He called me in early January 2010 and we discussed what I might do. He suggested submitting a proposal. The three key elements of the proposal were to be:

1. Evaluate the present status of the Multiphase Roadmap-give my opinion(s)
2. Make suggestions on how to modify the Multiphase Roadmap, i.e., what needs to be changed, added, deleted and why
3. Define the next step(s) to go forward—funding sources, organization, leadership

Syamlal responded and requested that I submit a 2 page proposal to perform the following tasks:

1. Evaluate the present status of multiphase flow modeling to determine the items in the Multiphase Roadmap that have been fulfilled and the items that remain to be done. Survey all the related work supported by NETL. Survey also related work supported by external national and international agencies;
2. Make suggestions on how to modify the Multiphase Roadmap so that the 2015 vision can be achieved, i.e., what needs to be changed, added, deleted and why;
3. Define the next step(s) to go forward - funding sources, organization, leadership;
4. Present the above information at the May Workshop (in Pittsburgh, PA) and lead a discussion with the meeting participants;
5. Summarize all the above information in a report to be submitted by the end of June 2010.

The areas of fossil energy application include:

- CO_2 capture,
- coal gasification, and pyrolysis,
- fossil fueled power plants including emissions control and reduction,
- coal cleaning and desulfurization,
- coal liquefaction, i.e. clean coal derived liquids for transportation and chemical feed stocks including a gas-liquid and/or gas-solid-liquid perspective,
- natural gas,
- oil sands,
- gas hydrates,
- oil shale, and
- fuel cells.

In early February 2010 Syamlal informed me that NETL was planning to go ahead with the project and that a contract would be put in place. This took until the end of March because of the change in the NETL contracting consultant firm from Parsons to URS. I then proceeded to prepare my presentation for May 4 at the 2010 Workshop on Multiphase Flow Science at the Pittsburgh Airport Marriott Hotel. Ray Cocco and I met on February 23 to go over my draft presentation and to get a preliminary assessment of the Multiphase Roadmap. A subsequent follow up meeting on April 20 with Ray and Ron Breault resulted in an extensive review with much give and take of my revised draft. This report fleshes out and expands upon my presentation and generally follows the same general format.

2 Previous Efforts at Multiphase CFD Roadmapping and Lessons Learned

"Those who cannot learn from history are doomed to repeat it."

George Santayana

"Insanity: Doing the same thing over and over again and expecting different results."

Albert Einstein

In order to place the Multiphase Roadmap into perspective, it is vitally necessary to trace the major events preceding its initiation in 2006. Valuable lesson learned are obtained from these events that should be useful to further the Multiphase Roadmap and to allow it to go forward in an orderly and successful manner in its goal for developing a useful, validated, and fast computer program for multiphase simulations. These lessons learned serve to form a good deal of the recommendation found in Section 5 "Recommendations and Path Forward". This accounting also serves to fills in gaps in the Introduction on page 12 of the Multiphase Roadmap report leading up to the Fluid Dynamics Research Consortium (MFDRC) which functioned from 1998 to 2003 and has not heretofore been documented.

At this point it is worthwhile to state the**Vision** of the Multiphase Roadmap as enunciated in the Multiphase Roadmap report [4]: to

"ensure that by 2015 multiphase science based computer simulations play a significant role in the design, operation, and troubleshooting of multiphase flow devices in fossil fuel processing plants."

I interpret this to mean power plants utilizing a variety of fossil fuels. This includes, but no limited to pulverized coal (PC) and fluidized bed combustion (FBC) boilers using coal, with and without oil, natural gas, and biofuels, as well as conventional and advanced coal gasifiers using atmospheric or pressurized bubbling or circulating fluidized beds.

2.1 A Time Line of Roadmapping and Workshops Relevant to Multiphase CFD and Lessons Learned

It must be recalled that multiphase flow research (or science) began in the nuclear power industry in support of safety analysis of the hypothetical loss of coolant accident (LOCA). The first three workshops below addressed issues hindering the development of this infant discipline.

1974 The very first Multiphase Workshop was the Round Table Discussion organized by Professor Dimitri Gidaspow at the Fifth International Heat Transfer Conference in Tokyo, Japan titled "Modeling of Two Phase Flow". Opinions on the issues of 1.) the state of development of the multiphase field equations, 2.) problems due to imaginary characteristics, and 3.) the direction that research should take. were invited from national and international leaders in multiphase flow research at the time and their written responses were summarized in the Proceedings [5]. [**Lesson learned**: This very first workshop demonstrated that cooperation among experts in disparate fields of multiphase flow research were willing to express their opinions openly and in print on important issues still relevant today.]

1976 Dimitri organized an NSF Workshop on Mathematical Modeling addressing 1.) problems with separate phase momentum balances and drift flux and 2.) scale up of coal conversion processes [6] [**Lesson learned**: research needs and recommendations should be identified on issues including: different forms of field equations, boundary conditions, reporting, diffusion coefficients, predictive capabilities, constitutive equations, critical flow, and use of linearized analysis, all issues still with us today.]

1979 EPRI held the Workshop on Basic Two-Phase Modeling in Reactor Safety and Performance, Tampa, Florida, February 27 – March 2, 1979. The list of participants is a Who's Who of experts in all phases of two-phase flow research at the time. In 1980 EPRI published a two volume Proceedings (EPRI WS-78-143) [7] containing transcripts of the discussions and presentations, some of which appeared in a special issue the International Journal of Multiphase Flow in 1980 (Vol. 6). [**Lesson learned**: Multiphase flow research is not an academic issue. It is of an international scope. Timely solutions must be address in an open manner with all opinions voiced. Transcripts of discussions may be of ephemeral nature but spontaneous and sometimes heated workshop participants' reactions can be quite useful and revealing]

1982 Two computer code developments were initiated under ERDA (now DOE) sponsorship: Systems, Science and Software (S^3) started work in 1975 on a general computer model of fluidized bed coal gasification called CHEMFLUB. JAYCOR started on a similar code in the early 1980's called FLAG. These two computer codes were transient and two-dimensional, contained partial differential equations (PDE's) similar to the ones contained in codes developed for analyzing nuclear reactor safety, and included viscous stress terms and expression for the solids pressure to keeps solids from compacting below the packed-bed state. In 1982 a workshop to review these two computer codes was held at Morgantown Energy Technology Center (METC) (now NETL) [8] and a contract was given to BDM Corporation to verify and document them. Smoot [9] and Gidaspow, in his D. Q. Kern Award Lecture, [10] reviewed the history of these efforts to which the reader is referred. [**Lessons learned**: the solids pressure term was developed and found to make the characteristics real in the limit of low fluid-phase volume fraction. Documentation is extremely important and should accurately describe what is in the computer program.]

1995 What really got the ball rolling for multiphase flow visibility and roadmapping on the national level was the DOE Office of Industrial Technology (OIT), now the Industrial Technology Program (ITP) Reactive Flow Simulation Multiphase Workshop hosted by Los Alamos National Laboratory (LANL), May 18 and 19, 1995 [11]. Several industrial companies were invited but no other National Laboratories. As expressed in the white paper prepared after the Workshop [12], the goal was to create a self-sustaining, fully-supported, constantly improving, comprehensive and substantially rigorous **computer simulation capability for complex multiphase dynamics problems which represents a quantum improvement over today's state-of-the-art.** This is to be comprehensive in the sense of enabling the partners to perform simulations necessary for their individual purposes, with a high level of confidence. The Virtual National Lab or Center of Excellence should also provide a conduit between fundamental and applied research. The idea and reasons for DOE virtual technology centers was outlined in an undated presentation by Dean Waters [13]. [**Lessons learned**: Wow. Such a virtual laboratory concept proposed for advancing multiphase dynamics was a tremendous idea. The intent of this concept was to maximize the return on the investment that the DOE has in its National Laboratories, and to serve as a model for moving other technologies from basic arena to the applied area. Such a Virtual National Laboratory would have embodied a Partnership among US government agencies including National Laboratories and Technology Centers, US private industries, US professional societies, and US Universities, all of which have a need for solving complex problems in multiphase fluid flow and/or material response, in order to control their processes, products, environmental impacts, and conservation of resources. Such a model would well serve the Multiphase Roadmap.]

1995-1996 On November 28, 1995 there was a follow up meeting, this time of representatives of all the National Laboratories, in Washington DC supported by DOE OIT. In the interim from the May meeting at LANL, the scope of the virtual technology center narrowed to a concept of a Virtual Multiphase Laboratory for the Chemical Industry. There was a growing perception at the National level that CFD computational technology, including multiphase flow, is critical to meeting the US chemical industry's future challenges. At this meeting the National Laboratory representatives presented overviews of their capabilities and agreed to look at common interests and working together in the area of multiphase flow. Also, it was agreed that the labs would attend the Dallas Team meeting in Dallas Texas December 13-14, 1995. The purpose of that meeting was to move through the National Laboratory Directors model for a Virtual Technology Center [13]. A Memorandum of Cooperation for the DOE Virtual Technology Center for Multiphase Dynamics (VCMD) was drawn up. It was intended to set forth the understanding among the Laboratories of the preferred processes for carrying out collaborative research and development. In that document were proposed a Coordinating Council, a schedule of Coordinating Council meetings (at least semiannually) and the role of industrial involvement. Starting in February 1996, I was given the task of preparing a document summarizing the National Laboratories multiphase capabilities in four categories: numerical methods, phenomenology and constitutive theory and modelling, experimental methods, and applications. In the process of preparing this document which took until December, 1996 Vision and Mission statements were developed [14].[2] The Vision 2020 Roadmap was being developed during this time period [15] [**Lessons learned**: It takes a considerable time to develop a coherent plan of attack and organization for a project of the magnitude proposed for the OIT Chemical Industry of the Future. In addition to a Vision statement which states **what to do**, a Mission statement needs to be

[2]By coincidence a similar report was produced in June 1996 by the Office of Energy Research and Development, Natural Resources Canada titled *Multiphase R&D in Canada.*

developed which defines **how to do it**. A memorandum of cooperation is necessary to clearly define the operation of collaborative research involving National Laboratories, universities and industry.]

1996 The National Workshop on Computational Fluid Dynamics and Multiphase Flow Modeling was held at the University of Maryland, October 30-31, 1996. This meeting consisted in the exchange of information between members of the chemical and high performance computer industries regarding need and future industry direction and development. Various DOE Program Offices expressed their interest in the area of Multiphase Computational Fluid Dynamics: the Office of Energy Efficiency and Renewable Energy, the Office of Energy Research, and the Office of Defense Programs. Representatives of the National Laboratories and academia presented their views on the state of the art and future technology development areas including a presentation of the National Laboratories Multiphase capabilities which at the time of this meeting was nearing completion. A roadmapping session provided input and detail into the previously identified set of projects of importance to the Chemicals Industry. Technology development and need was forecast over the next ten years. Input was arranged by the two major flow types, gas/solid and gas/liquid/solid flows. The technology need areas for these flow types were prioritized.[16] It took until January 1999 to finalize the Technology Roadmap for Computational Fluid Dynamics [17] which contained elements from this report defining the areas of multiphase flow requiring development: 1.) Numerical Methods, 2) Phenomenology and Constitutive Relations, and 3) Experimental Validation. Within these three areas, research needs were identified and given top, high, and medium priorities and time frames of near term (0 to 3 years), mid term (3 to 5 years), and long term (5 to 10 years). [**Lessons learned**: Multiphase flow research needs not only to be broken down by near, middle and long term but also by priorities of top middle and low. Once again the time it takes to produce a top quality roadmap takes a long time, in this case about three years from 1995 Los Alamos National Laboratory meeting.]

All of the above roadmapping and workshop effort developed into what became the Multiphase Dynamics Research Consortium (MFDRC), initiating at the kickoff meeting July 20-21, 1998 at Cray Research Headquarters in Eagan, Minnesota, hosted by Silicon Graphics. The MFDRC terminated in 2004 much to my surprise as there was no "sunrise" agreement ever discussed at the semi annual meetings. Although much progress was made, few of the goals set up in the Technology Roadmap for Computational Fluid Dynamics [17] were met, especially the development of a reliable and validated multiphase CFD code useful for the chemical industry.

1997-2007 The following important roadmaps and documents all have relevance to the Multiphase Roadmap. Some were referred to in the Multiphase Roadmap report but without their web links: They are listed here together with their web links for convenience of the reader to quickly download them.

Workshop Multiphase Flows and Particle Methods, 1997. [18]
Chemical Industry of the Future Technology Roadmap for Computational Chemistry (1999) http://www.chemicalvision2020.org/pdfs/compchem.pdf
Vision 2020 2000 Separations Roadmap (2000) http://www.chemicalvision2020.org/pdfs/sepmap.pdf
Vision 2020 Reaction Engineering Roadmap (2001)
http://www.chemicalvision2020.org/pdfs/reaction_roadmap.pdf
Workshop on Scientific Issues in Multiphase Flow (2002) http://multiphase.princeton.edu/SS_Publications/100.pdf
Clean Coal Technology Roadmap (2004)
http://www.netl.doe.gov/technologies/coalpower/cctc/ccpi/pubs/CCT-Roadmap.pdf
http://www.netl.doe.gov/technologies/coalpower/cctc/ccpi/pubs/CCT-Roadmap-Background.pdf
Clean Coal Technology Program Update 2009 (2009) http://www.fossil.energy.gov/programs/powersystems/cleancoal/publications/CCT_Program_Update_2009.pdf
IFRPI Powder Flow Working Group Report 2005 http://www.nsf.gov/eng/cbet/activities/IFPRI-powderflow-SAR30-08.pdf
IFPRI web site http://www.ifpri.net/default.asp
Report to the President 2005: Computational Science Ensuring America's Competitiveness (2005)[3]
http://www.nitrd.gov/pitac/reports/20050609_computational/computational.pdf
CO_2 Separation Technology (2007)
http://www.chemicalvision2020.org/pdfs/CO2_Separation_Report_V2020_final.pdf
Council of Industrial Boiler Owners web site http://www.cibo.org/links.htm
DOE Industrial Technology Program Areas linking to roadmaps
http://www1.eere.energy.gov/industry/program_areas/industries.html
Institute for Multifluid Science and Technology (IMUST) http://www.crss.ucsb.edu/imust Proposal for Research on the Science and Computation of Multiphase Flows
http://www.crss.ucsb.edu/imust/NERI-NRC-proposal.pdf
2006 Workshop on Multiphase Flow Research
http://www.netl.doe.gov/events/06conferences/mfr_workshop/index.html
NETL 2009 Workshop on Multiphase Flow Science http://www.netl.doe.gov/publications/proceedings/09/mfs/
NETL 2010 Workshop on Multiphase Flow Science http://www.netl.doe.gov/publications/proceedings/10/mfsw/

[3] I was pleased to find that this report used the George Santayana quote appearing at the beginning of this section in a somewhat different wording.

In summary just what did all of these workshops and roadmappings accomplish? 1, They identified many industrial PROBLEMS and NEEDS requiring solutions. 2. The DOE Funded CHEMFLUB (S^3) and FLAG code (JAYCOR) development to seriously attempted to provide a validated multiphase CFD tool using experiments as a means to solve these industrial PROBLEMS and NEEDS. 3. They clearly identified and documented the multiphase CAPABILITIES of the National Laboratories. 4. The MFDRC was initiated.

2.2 Major Multiphase Flow Conferences

Conferences and workshops concentrating on multiphase flow started on the heels of Dimitri's 1974 Roundtable Discussion. The first of these was the Two-Phase Flow and Heat Transfer Symposium-Workshop, Fort Lauderdale, Florida, October 18-20, 1976 which was published in four volumes in 1978 by Hemisphere as "Two-Phase Transport and Reactor Safety" [19]. This conference series continued as the Miami International Symposium on Multi-Phase Transport & Particulate Phenomena until 1988. The first International Conference on Multiphase Flow (ICMF) was held in Tsukuba, Japan, in 1991.and continued in the wake of the termination of the Miami International Symposium on Multi-Phase Transport & Particulate Phenomena in 1988. The second ICMF Conference was held in Kyoto, Japan in 1995 where it was decided the conference should be held every three years. ICMF 1998 was held in Lyon, France, ICMF 2001 in New Orleans, USA, ICMF 2004 in Yokohama, Japan, and ICMF 2007 in Leipzig, Germany. ICMF - 2010 is to be held in September 2010 sponsored by the University of Florida. Alternating with the ICMF conferences is the International Conference on Computational and Experimental Methods in Multiphase and Complex Flow. The first conference in the series was held in Orlando (2001), followed by Santa Fe, New Mexico (2003); Portland, Maine (2005), Bologna, Italy (2007), and the 5th in 2009 in New Forest, UK.

3 Summary of Major Successes of the MFDRC and the Multiphase Roadmap

> "As far as the laws of mathematics refer to reality, they are not certain; as far as they are certain, they do not refer to reality."
>
> Albert Einstein

This section will summarize selected major accomplishments of the MFDRC and projects funded by NETL which have fulfilled items listed in Chapter 5 of the Multiphase Roadmap report. [4]

3.1 Multiphase Dynamics Research Consortium (MFDRC) Successes and Failures

The following is my personal impression of the MFDRC successes and failures in my role as basically an outsider funded separately by Brian Valintine. Group A was better organized around the Sandia riser project than Group C which was interested in modeling cohesive powders. As far as I could see there was no direction of what should really be modeled (Sandia riser, IIT riser, NETL riser, Dow Corning experiment…) or by whom (IIT, Purdue University, Dow Corning, LANL, Sandia…) and with which code, (MFIX, CFDLIB, IIT, Purdue, FLUENT, CFX, Arena-flow…). The MFDRC participants would all come together, do their show and tell, argue about what should and could and could not be modeled and why, and then leave with no action items. Then they would reassemble six months later to do more show and tell as though there was no remembrance or recollection of the last meeting. The Arena-flow code representatives joined the MFCRC later in its existence. [20] It uses the multiphase particle in cell (MP-PIC) method which appears to have originated at LANL. Ray Cocco is of the opinion that he though that Arena-flow, now known as the commercial code BARRACUDA (see www.cpfd-software.com) was the most significant success to come out of the MFDRC. He told me this when I consulted him preparing for my May 4 presentation at the NETL 2010 Workshop on Multiphase Flow Science. [24]

CFDLIB sort of fell into oblivion after the MFDRC terminated, with no prospects for commercialization. MFIX was parallelized and chemical reactions were added. These features would have probably have added even without the MFDRC (MFIX started in 1991). At least MFIX is an open source code and is beginning to be used by researchers worldwide but probably not by engineers.

Tyler Thompson was instrumental in "selling" the MFDRC when he was Manager of External Projects at Dow Chemical and has a much more positive spin on its success. He has since retired and is currently on a nearly one year travel vacation. Surprisingly, he is not involved with the Multiphase Roadmap. I finally caught up with him via email while he was staying in England. What follows is my edited version of his take on what he felt were the major successes of the MFDRC.

The successes of the MFDRC (1998–2004) fall into two categories: technical and community. Technical successes include the following which were reported in monthly highlights and quarterly progress reports produced by Sandia National Laboratories (SNL) during the life of the consortium: 1.) Exploration of new phenomenological models by Brian (Bucky) Kashiwa at LANL, multiphase turbulence [21] and the development of the multiphase CFDLIB code. [11, 18, 22] 2.) Generation of valuable gas-solid flow data (the Sandia riser) and associated application of non-intrusive instrumental techniques and analysis on the Sandia riser. [22, 23]. and 3.) Significant code improvements in the MFIX: addition of chemical reaction and parallelization of the code with the assistance of Oak Ridge National Laboratory (ORNL) (see the MFIX web site https://mfix.netl.doe.gov). and 4.) Sophisticated applications of multiphase flow modeling within several of the participating companies, notably Dow Chemical, Dow Corning, Fluent, Millennium Chemical, and Exxon.

Tyler is actually more enthusiastic about the successes in developing the community, communicating and working together with each other for a sustained period of 7 year (1997–2004). He once made a slide listing all of the individuals and institutions that the consortium roped into this enterprise, including direct funded participants, cost-sharers, graduate students, post-docs, invited speakers at semi-annual meetings, and others who were somehow touched by the MFDRC. It amounted to over 200 professionals. The program that the DOE supported through these efforts had a lasting impact on the lives and careers of many of the most creative and productive scientists working in this specialized field of multiphase flow modeling. One of the most important lessons learned was how effective a self-organized, self-managed group of enthusiasts can be when they agree to **work together on a common challenging goal**. All it took was some faith and sustained funding from the government—money that the DOE would have spent anyway. But by funneling the MFDRC funding through the industry-led initiative, they encouraged the whole community to pay attention to the industrial needs, applications, and insights. The research was much better coordinated and more effective in addressing real problems than is typical of most government programs.

3.2 Multiphase Roadmap Successes

The successes of the so-called “external” projects funded by NETL are summarized in this section. External projects as explained to me by Ron Breault are those projects considered to be external to in-house or “internal” activities within NETL. Since the NETL internal projects are not required to write progress reports I cannot judge their success. Peer reviewed publications and conference proceedings might constitute success but I will not make that judgment. Successes of NETL’s external projects were determined by going through the progress reports kindly supplied to me by Ron Breault and Susan Maley of NETL and Christine Hryenya of the University of Colrado at Bolder. Ray Cocco kindly allowed me to access the web site of the following polydisperse flows project. Professor Sundaresan also supplied a summary of his external projects.

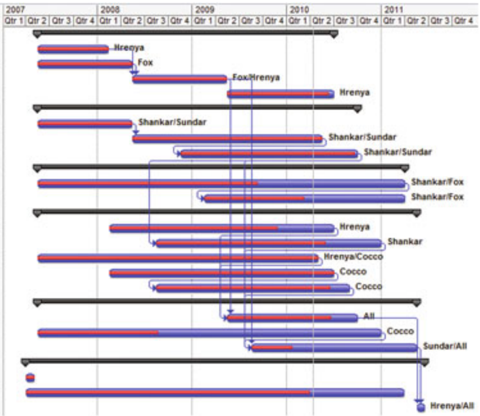
3.2.1 Development, Verification, and Validation of Multiphase Flow Models for Polydisperse Flows Project

This is by far the most organized and focused project funded by NETL vectored toward the Multiphase Roadmap. The principal reason for this is the organizational skills of Ray Cocco. He was the principal author of the Track 4 Section of the Multiphase Roadmap report. He was also the task master, so to speak, for the MFDRC. The principal investigator of this project is Prof. Christine M. Hrenya (University of Colorado) and the principal coinvestigators are Dr. Ray Cocco (PSRI), Prof. Rodney O. Fox (Iowa State University), Prof. Shankar Subramaniam (Iowa State University), and Prof. Sankaran Sundaresan (Princeton University). The overall aim is the development of first-principles, continuum models of *polydisperse* gas-solids flows for incorporation into MFIX and to carry out validations studies using both discrete-particle simulations and experiments. Polydisperse gas-solids flows are distinguished by solids having a particle size distribution. The technical goals of this 3-year project are: **Goal I:** Development of continuum theory for the solids phase **Goal II:** Development of gas-particle drag laws **Goal III:** Development of turbulence models **Goal IV:** Data collection and model validation. These goals encompass several near-term, mid term, and long-term research needs of the Multiphase Roadmap in all five categories. The Gannt chart for this project is shown in Table 1. There is a web site established to enable good communication for the participants to access progress reports, presentations and summaries of frequent teleconferences. A good measure of the metrics of this project are publications: 3 book chapters, 22 journal publications, p conference proceedings, 23 invited presentations and 30 conference presentations.

Most of the tasks have been completed successfully. For example: 1. Development and verification of a constitutive model for fluid-particle drag for bidisperse suspensions, generalization to polydisperse systems, and implementation in MFIX, and 2. Implementation of polydisperse kinetic theory (known as the GHD theory) in MFIX and testing. However, a one-year extension addressing model validation (Goal IV), with an emphasis on three-dimensional MFIX simulations has been requested. The two issues proposed to be addressed are: (i) the effect of

Table 1 Gannt Chart for the Polydispersed Flows Project

	Task Name	Start	Finish
1	**1. Goal I: Continuum Theory**	**Tue 5/15/07**	**Wed 6/30/10**
2	1.1 Derivation of KTGF	Tue 5/15/07	Wed 2/13/08
3	1.2 Development of DQMOM	Tue 5/15/07	Wed 5/14/08
4	1.3 Incorporation into MFIX	Thu 5/15/08	Thu 5/14/09
5	1.4 Extension of KTGF	Fri 5/15/09	Wed 6/30/10
6	**2. Goal II: Drag Laws**	**Tue 5/15/07**	**Fri 10/1/10**
7	2.1 LBM/DTIBM: zero vel.	Tue 5/15/07	Wed 5/14/08
8	2.2 LBM/DTIBM: non-zero vel.	Thu 5/15/08	Sat 5/15/10
9	2.3 LBM/DTIBM: freely evolving	Sat 11/15/08	Fri 10/1/10
10	**3. Goal III: Gas-Phase Turbulence**	**Tue 5/15/07**	**Fri 4/1/11**
11	3.1 DNS of poly., turb flow	Tue 5/15/07	Fri 4/1/11
12	3.2 Multiphase turb. Model	Mon 2/16/09	Fri 4/1/11
13	**4. Goal IV: Data Collection & Model Validation**	**Tue 5/15/07**	**Tue 5/17/11**
14	4.1 DEM: granular systems	Fri 2/15/08	Wed 6/30/10
15	4.2 Eulerian-DEM: gas-solid systems	Fri 8/15/08	Sat 1/1/11
16	4.3 Expt: Low-velocity bed	Tue 5/15/07	Fri 4/30/10
17	4.4 Probe development: clusters	Fri 2/15/08	Wed 6/30/10
18	4.5 Expt: High-velocity bed	Fri 8/15/08	Tue 8/31/10
19	**4.6 Model Validation**	**Tue 5/15/07**	**Tue 5/17/11**
20	4.6.1 Validation: CU Expt. & DEM Sim.	Fri 5/15/09	Thu 9/30/10
21	4.6.2 Liaison to NETL experiments	Tue 5/15/07	Fri 12/31/10
22	4.6.3 Validation: NETL/PSRI Expt. & Eulerian-DEM Sim.	Mon 8/17/09	Tue 5/17/11
23	**5. Goal V: Project Management**	**Sun 4/1/07**	**Thu 6/16/11**
24	5.1 PMP	Sun 4/1/07	Tue 5/1/07
25	5.2 Progress Reports	Sun 4/1/07	Wed 3/30/11
26	5.3 Final Report	Wed 5/18/11	Thu 6/16/11



polydispersity on clustering, and (ii) comparison of predictions from polydisperse simulations with the PSRI experimental data.

3.2.2 Princeton University Projects

Closures for coarse-grid simulation of fluidized gas-particle flows

The goal of this project is to develop a filtered two-fluid model that can be used to carry out coarse-grid simulation of gas-particle flows, along with all the closure relations needed for the filtered model; verify the fidelity of the filtered model by comparing its predictions against highly resolved simulations of a kinetic theory based model; and validate against experimental data. The successes have been: 1. Development and verification of a filtered two-fluid model for the flow of uniformly sized particles along with the required constitutive models. This model is limited to dilute flow where the particles interact predominantly through binary collisions. 2. Development of wall corrections for the constitutive models, and 3. Comparisons with experimental data in the literature for validation. This project has been completed and the final report is under preparation; one manuscript has been published and 3 more are in preparation. This project involved participation of Drs. Sreekanth Pannala, Thomas O'Brien and Sofiane Benyahia of NETL

Rheological behavior of dense assemblies of granular materials

The goal of this project is to develop and validate constitutive models for frictional, quasi-static flow which capture the essential features of the plastic regime, and the transition to the intermediate and rapid flow regimes. The successes have been: 1. Development and verification of a constitutive model for the quasi-static flow regime that incorporates the evolution of microstructure in the stress model which expresses macroscopic stresses in terms of particle scale properties, and 2. Identification of the asymptote which serves as the attractor for the stresses in the intermediate regime. This asymptote depends on particle scale friction coefficient and is blended with the quasistatic and inertial regime rheology to obtain a comprehensive rheological model. Work is in progress to implement it in MFIX. This project also involved Professors Gaby Tardos (CCNY) and Shankar Subramaniam (Iowa State). This project is now in a no-cost extension. Two manuscripts have been published and 3 more are in preparation.

These two projects encompass several near-term and mid term research needs of the Multiphase Roadmap in the Benchmark Cases, Numerical Algorithm and Software Development, and Theory and Model Development categories.

3.2.3 Development of Criteria and Identification of Particle Cluster Size Based on Measurements of Void Fraction in Gas-Solid Systems

The objectives of this project at the Florida International University were to 1. Apply advanced experimental techniques and develop a new mathematical analysis procedure to identify particle cluster size, based on measurements of void fraction, in gas-solid flow structures in risers and vertical columns; 2. Generate detailed experimental measurements necessary for CFD validation; modify existing correlations describing the hydrodynamics of gas-solids systems; 3. Expose minority

Table 2 Gantt Chart for the Florida International University Project

Task Description	Time	Start	End	Status ASOF 12/31/08
Task 1- Develop Project Management Plan	23 days	1/1/2007	1/31/2007	Completed
Task 2- Experimental setup and testing of circulating fluidized bed riser	244 days	2/1/2007	1/8/2008	Completed
Task 3- Configure and test shadow sizing system	65 days	7/30/2007	10/26/2007	Completed
Task 4- Experimental data collection	75 days	1/9/2008	4/22/2008	Completed
Task 5- Image analysis to obtain velocity and void measurements	113 days	1/23/2008	6/27/2008	Completed
Task 6- Identification of void fraction associated with maximum granular temperature	45 days	03/09/2008	06/08/2009	In progress.
Task 7- Mathematical analysis of collected data to identify criteria for cluster size	10 days	06/08/2008	06/20/2009	In progress.

students to scientific research in the field of fluid dynamics of gas-solids flow systems; and maintain and upgrade the educational, training and research capabilities. It appears to have terminated on June 30, 2009. Table 2 summarizes the limited successes made up to that date

3.2.4 Dense Multiphase Flow Simulation: Continuum Model for Poly-Dispersed Systems Using Kinetic Theory Project

The goal of this project at the University of Puerto Rico – Mayaguez is to develop the kinetic theory for poly-dispersed systems based on a unique particle size and velocity distribution function using the generalized Boltzmann equation (GBE) through a generalized method of moments (GMOM). The Finite size domain Complete set of trial functions Method Of Moments (FCMOM) technique developed at the Illiois Institute of Technology will be used. [25] The resulting equations will be incorporated in MFIX, and will significantly improve this code for realistic prediction of flow patterns and particle evolution in coal conversion and gasification processes. The success of this project appear to be limited. It is not clear if this three year project is continuing to complete its proposed tasks

4 Review of the Multiphase Roadmap Report

This section is my review of the Multiphase Roadmap report. [4] I reviewed it as though it were a manuscript sent to me for review for a peer reviewed journal publication. I applied my usual constructive criticism criteria.

First I was struck by the cover of the Multiphase Roadmap report. At a Metal Wastage Review Meeting held at METC on May 17, 1988 I had proposed the MACRO/MICRO Modeling approach to analyze erosion in commercial fluidized bed combustors as shown in Figure 1.

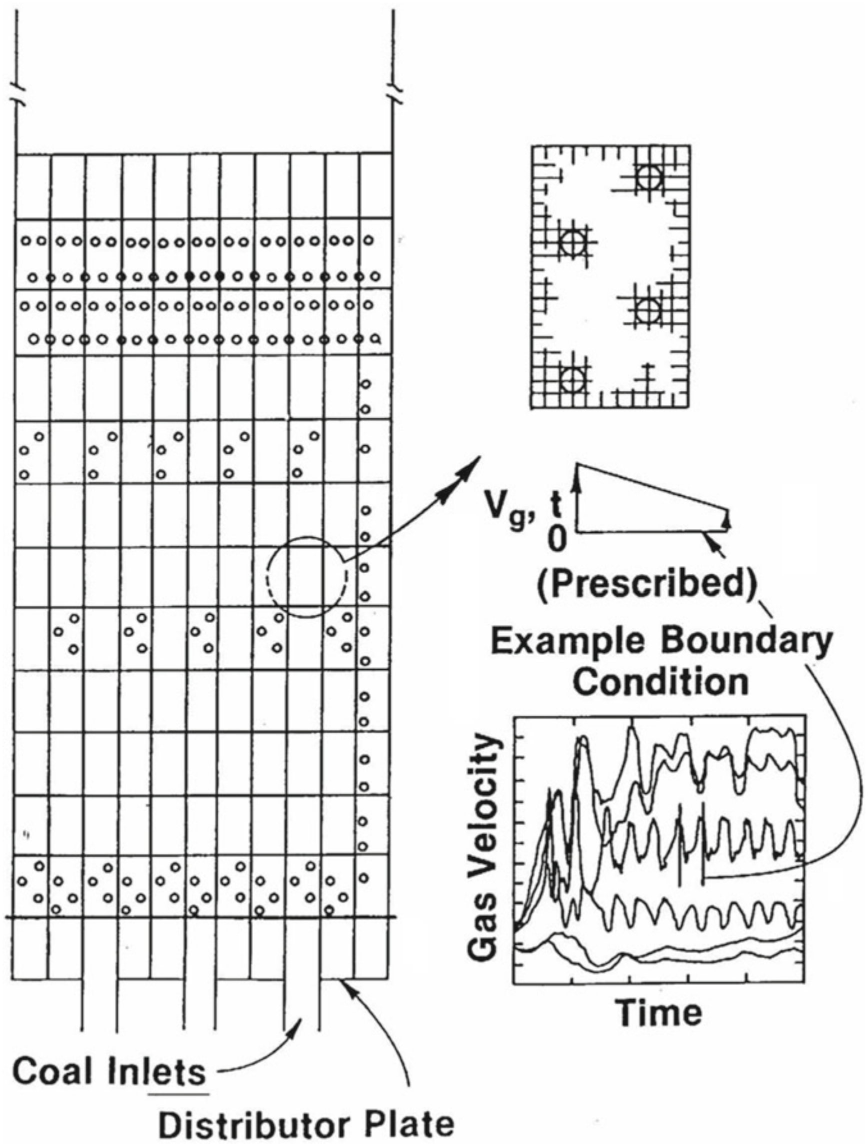


Figure 1 MACRO/MICRO Procedure for Modeling Hydrodynamics and Erosion in Large-Scale Fluidized Bed Combustors

What was proposed was to model the large-scale macro geometry with a distributed resistance model for the water cooled tubes which carry away steam to the turbines. In this model the individual tubes are averaged out and replaced with a drag function. The reason for such a model is that it is computationally prohibitive to model each and every one of the hundreds or thousands of tubes. Then selecting a unit cell of tubes, a micro-scale calculation for the hydrodynamics and erosion would be performed using as a driving function the inlet gas velocity computed over one cycle during which limit cycle had been established. The reaction as I recall was that this was an intriguing idea but too filled with risk and so it was abandoned from the project.

4.1 Specific Comments

1. Pages iv - vi: The telephone numbers and emails of participants, other contributors should have been added.
2. Page vi: The affiliations of the industry chairs and University co-chairs should have been added to the matrix.
3. Page 2 first full paragraph: "Second, although desirable, it is not certain that the same software can be used for describing different types of flows (gas-solids, gas-liquid, gas liquid-solids) or even for different flow regimes within a particular type of flow (dense and dilute in gas-solids flow; bubbly flow, plug flow, stratified flow, and slug regimes in gas-liquid flow)." I believe that not only that the different types of flows it can be described within the same software but it must be done. Otherwise you wind up with a series of codes that will confuse the user. With proper constitutive equations and drop down menus like in ANSYS FLUENT or COMSOL these flows are easily accommodated. As far as flow regimes, three-dimensional flows will evolve them naturally.
4. Page 4 third to last paragraph. The transition from Geldart group B to A is natural [26], however it may depend somewhat on the solids elastic modulus.
5. Page 4 second to last paragraph: I suggest that the erosion be moved to near-term need and that the MED erosion model be used (see APPENDIX A).
6. The proposed collaboratory was proposed but is now not an integral part of the Multiphase Roadmap. Was this in response to outcries at the 2006 workshop? In an email query to Syamlal, his answer was that "The roadmap was supposed to guide the collaboratory, proposed in the white paper (reference [26] in the Multiphase Roadmap report-RWL). The collaboratory concept did not workout as imagined in that document. But we have been able to focus NETL supported multiphase research using the roadmap."
7. page 11 first full paragraph: Reference [38] might better be used at this point where the quote occurs. Reference [8] is probably needed however, at the top of page 13 because the details of the workshop are deleted but the quote there (which I find baffling) is also in reference [38]. Sunderesan sent me reference [8] but it is dated December 2002 so there may be some confusion as to the date.
8. page 11 second full paragraph: Appendix B is referred to before Appendix A on page 14. This should have been corrected.

9. page 14: the first full paragraph is redundant since it repeats the first paragraph on page 1.
10. Page 17 first paragraph. Reference [18] should be reference [25].
11. Page 22: Reference [121] is out of sequence, last previous reference is [25] (in error as reference [18] on page 17). As an aside just why is this figure here? Perhaps it should have been moved to the Summary which first refers to Geldart group B and A on page 4..
12. Page 26: The jump to reference [118 fourth line from the bottom of the first paragraph is out of sequence; the last reference before this one is reference [67].
13. page 30 item 1.: Enwald et al. [27] compared several drag laws and showed that they all give about the same values over the entire range of solids volume fraction up to the packed bed state. On another issue, industry will be quite protective of their industrial scale data and will be unwilling to part with it so as not to help the competition. An exception to this rule was the cooperative development of fluid catalytic cracking during World War 2. by several oil companies together.
14. Page 34: In item 6 under Experimental, the authors are unaware of the experiment and modeling that was done using the computer-aided particle-tracking facility (CAPTF) experiment for a thin bubbling fluidized bed containing simulated imbedded heat transfer .tubes. [28]
15. Page 37: What is a stirred tank simulation doing in track 2 discussion? It should have been moved to page 43 and the simulation of airflow in a lung removed!
16. Page 45: "specific objects" should be "specific objectives" under Recommendations
17. Page 46 third full paragraph: Fluidized bed combustion is a *newer* technology? Certainly not newer than FCC.
18. Page 47. At the start of the background, the authors fail to mention COMSOL, PTAK, Star-CD and Flow-3D. They also fail to mention available K-FIX.
19. Page 37: The authors fail to realize that COMSOL has exactly the feature they describe to allow incorporation of various constitutive equations, and solvers using a GUI that looks very similar to Figure 4.3 on page 56.
20. Page 62. Four categories are listed by bullets but Benchmark Cases in the matrix on page 63 is missing! The sentence below the bullets sort of warn us what to expect next.

4.2 General Comments

1. Chapter 1 is rather sketchy. It appears to be identical to the track 1 draft report. The simplified Gannt chart on page 20 actually goes significantly beyond 2015 (blocks C and D)!
2. Chapter 2 is quite good with priorities assigned as high, medium and low. It appears to be identical to the track 2 draft report. Unfortunately, no Gannt chart is given. The implication of "pragmatic" is elusive. In the block diagram on page 30, the authors imply that pragmatic applies to modeling industrial-scale reactors with less rigor than validation experiments.

3. Chapter 3 is by far the weakest of all four tracks. None of the material from the summary nor Dudukovic's presentation were factored in.
4. Chapter 4 is the best thought out of the four tracks because Ray Cocco told me he wrote it. It is superior to the other three track plans for the reasons discussed in Section 3.2.1 Development, Verification, and Validation of Multiphase Flow Models for Polydisperse Flows Project.
5. Chapter 5 Pages 62-67: Now come the coups de grace: the biggest hurdle to comprehending the organizational structure of the Multiphase Roadmap report. The discussions in Chapters 1 through 4 are organized by the four tracks: 1. Dense gas-solids flows and granular flows, 2. Dilute gas-solids flows, 3. Liquid-solids and gas-liquid flows, and 4. Computational physics and applications. Suddenly we have the research needs from these four tracks somehow remapped into five categories: Benchmark Cases, Numerical Algorithm and Software Development, Theory and Model Development, Physical and Computational Experiments, and Communication, Collaboration, and Education.

4.3 Discussion and Summary

Is it Multiphase Research or Science that the Multiphase Roadmap is trying to advance? The Multiphase Roadmap report was called Workshop on Multiphase Flow **Research**. The 2009 and 2010 workshops are called Workshop on Multiphase Flow **Science**. Or is it **Engineering**? Professor Dudukovic emphasized in his 2010 Multiphase Workshop Plenary presentation [29] that **science is about knowing, engineering is about doing**.

The Multiphase Roadmap in its present form is far from complete. The organizers and participants did not go through the rigorous procedures established by the DOE employed in the production of its numerous roadmaps. In addition it is confusing. The reader is expected to try to map the four tracks discussed in Chapters 1 through 4 into the five categories presented in Chapter 5. The example shown in Table 3, taken from the National Workshop on Computational Fluid Dynamics and Multiphase Flow Modeling [16] illustrates a better way that could have been used to organize multiphase research needs. Each track should have been represented by a separate table with the identified research needs organized into the categories. In this way the continuity from the previous four chapters would have been preserved. The priorities from track 2 are missing and the other three tracks failed to identify any. The priorities should have been clearly identified for all four tracks and incorporated as indicated in Table 3.

There is no industry buy in of any kind and no industrial problems identified. What industry is associated with fossil energy anyway, boiler manufacturers (CIBO), EPRI, the coal industry? There are very few if any PC power plants being built in the USA. FBC and CFBC plants are commercially available. To my surprise the International Conference on Fluidized Bed Combustion annual meetings ceased about half a dozen years ago. Does this mean that all problems have been satisfactorily solved?

The impression running through the Multiphase Roadmap is that although NETL wants to model and help develop advanced circulating bed gasifiers for power

Table 3 Table II for Gas-Solids Flow Systems Roadmap [16]

Table II: GAS/SOLIDS FLOW SYSTEMS ROADMAP			
Numerical Methods:	**0–3 Yrs**	**3–5 Yrs**	**5-10 Yrs**
Dense phase modeling - I, II, III	xxx*	xxx	xxx
Validation and scaling - I, II, III	xxx	xxx	xxx
Complex geometry - I, II, III	xx	xx	xx
Adaptivity - I, II, III	xx	xx	xx
Parallelization - II, III	x	xx	xx
Chemistry, chemical coupling - I, II, III	x	x	x
Flow regime transition (numerical bifurcation) - I, II, III	x	x	x
Optimization - II, III		x	x
Phenomenology and Constitutive Relations			
Interactions between phases - I, II, III	xxx	xxx	xxx
Reliable turbulence closure for multiphase - I, II, III	xxx	xxx	xxx
Chemistry models (volume, surface) - I, II, III	xx	xx	xx
Boundary conditions - I, II, III	xxx	xxx	xxx
Population balance - III			x
Experimental Validation			
Validation at small scale - I, II, III	xxx	xxx	xxx
Separate effects - I, II, III	xxx	xxx	xxx
Analysis of results for non-linear systems - I, II, III	xx	xx	xx
New experimental methods applicable at large scale - II, III		xx	xx
Diagnostics and sensors - I, II, III	xxx	xxx	xxx

*Key: Top priority - xxx, Middle priority - xx, Lower priority – x

production via chemical looping, oxy-combustion, oxygen-free gasification using coal, biofuels, oil shale, etc., it would also like to expand its horizons to other fields of application like the chemicals industry. This is quite clearly stated in the white paper for the collaboratory for multiphase flow research (CMFR) [30] kindly supplied to me by Syamlal. It is also implied by the presence of 2 representatives from Exxon Mobil at the 2010 Workshop on Multiphase Flow Science.

There is an over concern about accuracy. Much emphasis is placed upon high accuracy, high fidelity computations. One must first determine the error bands of the data to see if such accuracy is warranted. Just how accurate one needs to be is entirely dependent upon the accuracy and reliability of the data extracted from validation experiments and industrial equipment. In the words of Pierre-Simon de Laplace, “The solution…depends…upon the accuracy of the observations and upon the perfection of the analysis.” [32] It is important firstly to predict correct trends. If the trends are wrong, then here is something seriously wrong with some model(s) which need to be critically reexamined. There is limited emphasis and definition of development of really simple experiments that test 1 or 2 sub-models, e.g., collapsing bed experiment, critical granular flow or comparison with closed form solutions such as found in Gidaspow’s book [33].

5 International and National Multiphase Research - Universities and Laboratories

It took me nearly a year working about half time to gather together the multiphase capabilities of the US National Laboratories [14]. An inventory of multiphase flow R&D in Canada documented the multiphase flow research capabilities at Canadian universities, government laboratories, and industrial laboratories took a similar amount of time. [31] Although these two documents represent capabilities as of 1996, surely they still have some relevance today. To update these two documents and to extend them to survey international universities, research laboratories, and industries multiphase activities would be very useful. However it would take much more time and effort than the time allotted for the present project. Professor Todd Pugsley of the University of Saskatchewan is interested in updating the Canadian survey and will contact of any progress. Therefore I will simply list the major institutions and individuals that I am aware of that I know are involved with various aspects of multiphase activities. For more, the reader is invited to visit the web site of the NETL 2010 Workshop on Multiphase Flow Science http://www.netl.doe.gov/publications/proceedings/10/mfsw/.

International Multiphase Research - Universities

Chalmers Institute of Technology – Sweden (A. E. Almstedt)
Imperial College – England (D. B. Spalding, B. van Wachem)
Lappeenranta University of Technology – Finland (T. Hyppanen)
Harbin Institute of Technology – China (Lu Huilin)
Chinese Academy of Sciences – (Jinghai Li)
Twente University of Technology (W. P. M. van Swaaij)
University of Pisa – Italy (A. Neri)
University of British Columbia – Canada (J. R. Grace)
Telemark Institute of Technology – Norway (E. Manger)
Osaka University – Japan (Y. Tsuji)
University of Melbourne (M. R. Davidson)

International Multiphase Research - Research Laboratories

Atomic Energy of Canada – Pinawa, Canada (W. T. Hancox)
Centre d'Etudes Nucleaires Grenoble – France (J. M. Delhaye)
CSIRO – Australia (Peter J. Witt, Y. Feng)
AERE Harwell – England (G. F. Hewett)
Institut de Mecanique de Fluides de Toulouse (Simonin)
International Atomic Energy Agency

National Multiphase Research - Research Laboratories

Los Alamos National Laboratory
Sandia National Laboratory
Pacific Northwest National Laboratory
Argonne National Laboratory
Lawrence Livermore National Laboratory

Idaho National Laboratory
Brookhaven National Laboratory
National Energy Technology Laboratory (NETL)
Particulate Solid Research Inc. (PSRI)

National multiphase research - Universities

Illinois Institute of Technology (D. Gidaspow, H. Arastoopour)
Rensselaer Polytechnic Institute (R. T. Lahey, D. B. Drew)
University of Texas at San Antonio (E. Michaelides)
University of California Santa Barbara (S. Banerjee)
University of Florida (J. Sinclair Curtis)
University of Colorado (C. Hrenya)
Princeton University S. (Sundaresan)
Purdue University (V. H. Ransom)
Ohio State University (L. S. Fan)

6 Recommendations and Path Forward

6.1 Research Needs

The monolayer energy dissipation (MED) erosion model described briefly in Appendix A is suggested to fulfill the long-term goal in the Theory and Model Development category in the Multiphase Roadmap. The (MED) erosion model is can use outputs from the MFIX computer code. This model has already been used successfully by Chalmers University [34] and Harbin Institute of Technology [35] to analyze erosion validation experiments.

There is no gas and liquid solids modeling or dense slurry modeling in the Multiphase Roadmap. This is a result of the inadequate input from track 3. Appendix B contains a fairly well laid out plan (when it was written some ten or more years ago) to study dense suspension flows. This plan was proposed for the Suspension Advanced Research Objective (SARO). This proposed project would have been a follow on to the Granular Theory Advanced Research Objective (GTARO) funded by the DOE. Unfortunately the SARO was not funded.

Additional recommendations include the following. 1. Bridge the transition between granular theory and Euler- Euler model. The models for solids pressure and viscosity should be consistent, 2.) Add particle rotation modeling component to complement the particle rotation visualization. 3.) Move ill-posedness of continuum equations from long range to near-term. This long standing issue must be resolved in a timely manner since it may be clouding the computations. 4.) Add spectral analysis and deterministic chaos modeling since it is extremely useful for understanding and reducing the massive time series outputs from computations 5.) Beef up the cohesion modeling effort. This was the thrust of a nearly successful proposal to NIST involving Dow Corning, Fluent, Inc., IIT, and Argonne National Laboratory. 6.) Develop challenge problems with close collaboration of modelers. Data not to be shown until results tallied. 7. All simulations should be done using MFIX with the same equations, submodels, geometry, nodalization (number, type), time step, numerical solver. 8.) The Cartesian mesh in MFIX should be extended to unstructured meshes. 9.) Develop fast running "averaged" equations capturing the essence of the physics. 10.) Update the National Laboratories multiphase capabilities [14] and get them involved in the Multiphase Roadmap[4], 11) Utilize the Sandia riser with its attendant nonintrusive instrumentation to complement PSRI's riser experiments. 12.) Pursue external funding and collaborative research with

- DOE Office of Science
- DOE ARPA E
- EPRI
- NASA
- DARPA

[4]Ron Breault appears to have done some sort of national and international survey of multiphase capabilities/needs for the 2006 Workshop on Multiphase Flow Research called International Energy Agency (IEA) Gap Analysis which may be utilized.

- NSF
- Council of Industrial Boiler Owners (CIBO)
- Other industrial sponsors

6.2 Multiphase Roadmap Management

High (H), medium (M) and low (L) priorities must be added to the Multiphase Roadmap. These priorities were developed for track 2 but never transferred. A Gannt chart for the entire Multiphase Roadmap is an important omission which must be rectified. It should show decision points and deliverables. The Gannt chart developed for the Polydispersed project shown in Table 1 is a good model.

A Mission statement and memorandum of cooperation such as developed for the VCMD [14] needs to be added. There should be established a steering committee to keep detailed track of direction and progress and a designated chairman who is in clear charge (although Syamlal appears to have a great deal of influence). An independent assessment of progress in the form of an external advisory committee must also be added. More metrics need to be added n addition to the three identified in track 4.

A clear statements as to the industrial problems to be addressed in the Multiphase Roadmap needs to be developed. NETL interacts with a multitude of industries involved with fossil energy, yet only non-fossil industry representatives were involved in the planning of the Multiphase Roadmap.

The model for CFD modeling methodology shown in Figure 2 was developed by the late David Davidson for Solutia. It is suggested as a paradigm for managing the Multiphase Roadmap and keeping it tethered to reality. I apologize for the poor quality of the figure obtained from a pdf of his presentation. Successful application of CFD requires three elements, 1. high performance computer hardware, 2. high performance CFD software, and 3. skilled practitioners as shown in the CFD Triangle. The industrial problem solving perspective figure below the CFD triangle illustrates the process whereby once the problem is resolved (the dotted line in the figure) there is no need to pursue the problem further. As far as industry is concerned, the residual uncertainties, while requiring additional work, become of academic interest and produce little or no immediate return and adds no additional value. That is to say, research produces a negative rate of turn on investment.

The practitioner's approach to the application of CFD is illustrated in the third figure. The customer identifies a problem from which the relevant physical phenomena are identified. The modeling experts then analyze and simulate the physical phenomena to design a practical solution that will correct the problem. A key ingredient in this process is the ability of the modeling expert to identify the *essential* physical problem that must be solved by CFD, and to solve only that problem. Commercial CFD codes are very powerful tools with extensive capabilities. However, Solutia found that the more of these capabilities one applies to a given problem, in general the less tractable the problem becomes. Only the capabilities that are *essential* to solution of the *essential* problem are requires. To attempt to solve every problem with unneeded complexity just because the code will allow you to do so is at the least inefficient and time consuming, and at worst leads to frequent failure. Furthermore, Solutia found it advisable to apply simpler methods, such as scaling analysis and analytical mathematics, whenever possible.

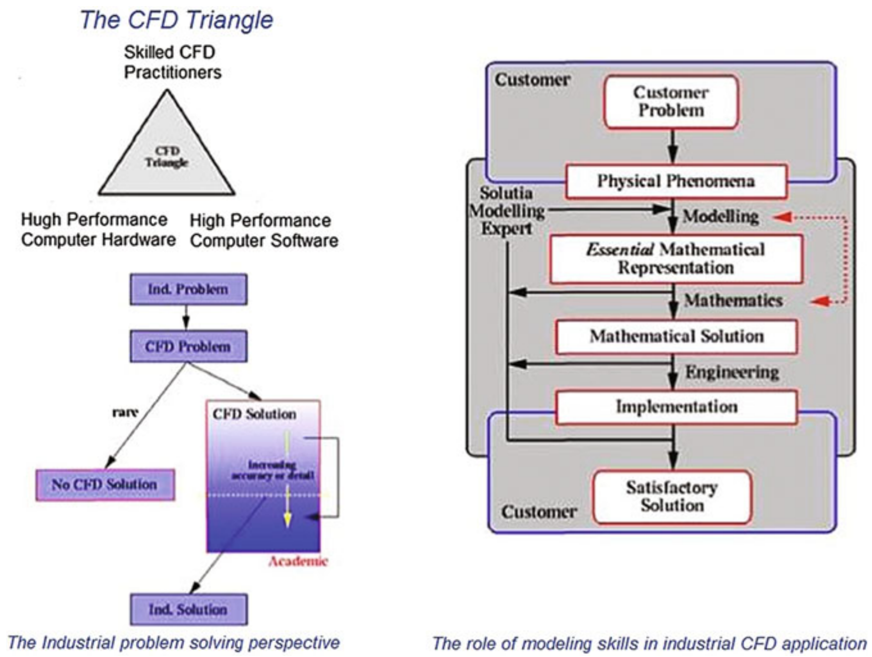


Figure 2 Industrial CFD Modeling Methodology Adapted from [36]

Tyler Thompson summed it up quite eloquently. "…my bottom-line lesson would be this: If you want a technology roadmap to be effective and really make a difference, it is essential to get industry scientists (T would add engineers-RWL) engaged. Unfortunately, that has become much more difficult in recent years. The research-oriented companies have tightened up and shrunk so much that industry scientists rarely have time or license to participate in the way that we did 1997–2003. I sense that the mood among management has become totally 'nose to the grindstone' - meet your immediate research goals - don't waste time on 'rising tide floats all boats' projects."

Communication needs a great deal of improvement. Track 4 made many recommendations, none of which have been implemented. Firstly there should be more frequent meetings, semiannual at least, quarterly would be better. Establish a web site making all presentations, reports, and memos available to all registered participants. This could be accomplished by adding to the MFIX web site or by combining and expanding the three web sites for the 2006, 2009, and 2010 workshops. Good communication is the key to success or failure. The collaboratory was an integral part of the Multiphase roadmap and is now totally independent from it. It should be folded iback into the Multiphase Roadmap.

Appendix C contains the 10 questions posed in my presentation at the 2010 Workshop on Multiphase Flow Science [24] together with the answers supplied by the only participant responding.

APPENDIX: Some Modest Proposals

A. MED Erosion Model

The definitive form of the MED erosion model is [37]:

$$\dot{E}_{ED\alpha} = (1 - e^2)U_{ED\alpha}/p = (1 - e^2)E_{ED\alpha}d_p/p \tag{A.1}$$

with α = 1, v, vCF, and vREL, respectively.

These MED erosion models are based on the premise that the mechanical energy of the solids is irreversibly dissipated in the neighborhood of stationary surfaces by three competitive mechanisms: 1.) heat transfer between the fluid-and-solids phase, between the fluid-phase and stationary surfaces, and between the solids-phase and stationary surfaces; 2.) erosion of stationary surfaces; and 3.) attrition of solids. Thus the rate of energy dissipated during erosion represents only a fraction of the total energy dissipation (which is related to the total entropy production).

The recommended MED erosion model, is given by:

$$\dot{E}_{MED} = (1 - e^2)[(\varepsilon_s\overline{\overline{\tau}}_{sv}) : \nabla\vec{v}_s + \overline{\overline{\beta}}_B\vec{v}_s^2/2]d_p/p = \dot{E}_{EDvCF} \tag{A.2}$$

The erosion rate from the simplified quasi one-dimensional MED model, $\dot{E}_{EDCF}$, may be written in the form, modified for hydrodynamic model B as

$$\dot{E}_{EDCF} = \dot{E}_o\frac{(1 - \varepsilon)(\varepsilon - \vec{\varepsilon}_{gd})}{\varepsilon^2} + K\frac{(\varepsilon - \varepsilon_{gd})}{\varepsilon^2}(U - \varepsilon V_s) \tag{A.3}$$

where the erosion rate group, $\dot{E}_o$, is given by

$$\dot{E}_o = (1 - e^2)\frac{75\mu_g g x_d}{(\phi_s d_p E_{sp})} \tag{A.4}$$

and

$$K = (1 - e^2)\frac{0.875 g x_d \rho_g}{E_{sp}} \tag{A.5}$$

The units of E_0 are in terms of a velocity; e.g., mm/1000 h and K is dimensionless.

In the above,

μ_g	gas viscosity, Pa·s
g	acceleration due to gravity, m/s^2
x_d	characteristic distance, m
d_p	particle diameter, m
Esp	an erodent (target) material property related to hardness, Pa
e	coefficient of restitution, ratio of rebound and approach particle velocities

ε porosity (fluid volume fraction)
ε_{gd} porosity in the densest region of the bed
ϕ_s particle sphericity
U superficial gas fluidizing velocity, m/s
V_s solids velocity, m/s

B. Concentrated Slurry Research Program Development

Concentrated solids-liquid suspensions have been studied little in the past. The conservation laws and constitutive relationships (power law, Bingham plastic, etc.) were generally modeled using a homogeneous continuum description for the phases. There have been very few direct evaluations of the various components such as solids and fluid fluxes, pressures, and stresses using fundamental data.

In this proposed study, a self-consistent volume- and time-averaging formalism[1] will be used to ('define the experiments and data required, and to develop and validate the conservation equations and constitutive relationships describing the phases. This proposed approach has the following unique advantages:

1. Clearly identifies parameters needed to be measured.
2. Provides direct linkage between microscale solids motion and interactions (solids-solids, solids-fluid) and macro-characterization of concentrated solid suspension such as stresses, fluxes, etc.
3. Evaluates the relative importance of each component (fluxes, pressure, stresses, and body force).

Once the parameters to be measured have been identified, this approach defines a clear path in the development of experimental measurement techniques and experimental facilities. Based on our preliminary investigation, in order to quantify various components for the solid suspensions, we need instantaneous local fluid and solids velocity (mean plus fluctuation), pressure distribution around solids, and characterization of collision of solids. NETL will develop necessary measurement techniques complementary to university partners to measure the needed parameters. In addition, the experimental slurry piping facility will place particular emphasis on studying the effects of elbow and flow splitter on the behavior of concentrated solid slurry. The ANL program will also conduct feature experiments of solids collision behavior. Parallel to the theoretical formulation and experimental efforts, NETL will coordinate and integrate the research work carried out by university partners and develop a consistent set of constitutive relations which will be used in MFIX developed by NETL for design and optimization of concentrated solids liquid slurry piping systems.

Reference:

1. J. G. Sun, *Analysis of Solids Dynamics and Heat Transfer in Fluidized Beds,* Ph. D. Thesis, University of Illinois at Urbana-Champaign (1989).

R&D RECOMMENDATIONS FOR CONCENTRATED SUSPENSIONS OF SOLIDS IN FLUIDS

The following summarizes the results of an extensive review of R&D needs and alternative research approaches for addressing the transport of highly loaded suspensions. This work is based upon meetings with groups of experts in this field, extensive technical discussions with individual investigators, and reviews of key articles and texts.

RESEARCH APPROACHES

I. Theoretical Studies

Theoretical work is required to establish the equations that govern suspension flows and to derive expressions for the transport coefficients that appear within the governing equations.

A. Transport Equations

Although there has been considerable research on multiphase flows, there is not yet a well-established set of governing equations for the flow of a highly-loaded solid-liquid suspension. At present, there exists a number of “physically reasonable” equations that have been proposed, and often vigorously defended, by various researchers. Much of the theoretical research effort appears to be expended upon examining the consequences of a particular set of transport equations, and insufficient effort is directed at resolving disparities and establishing a preferred set of governing equations.

The objective is to establish governing equations that would be analogous to the Navier-Stokes equations for simple fluids. There are three general approaches that are used for deriving continuum field equations for fluid transport: phenomenological theories, kinetic theories, and statistical mechanics.

Phenomenological Theories:

Almost all theoretical work in suspension flow has been based upon various phenomenological approaches. As a group, these approaches start with the macroscopic conservation equations for mass, momentum and energy. The differences among the various phenomenological approaches are in how each approach describes the suspension and formulates the constitutive relations that describe the response to gradients and forces. One class of approaches consists of modeling the suspension as a “single fluid” (e.g., a generalized / Newtonian liquid with a linear stress/deformation rate relationship) with a viscosity that is dependent upon the solid concentration. These assumptions establish the constitutive equation for momentum transfer. For mass transfer, this single-fluid approach allows the solid particles to move relative to the liquid, with a constitutive relation that models solids migration in response to density, shear and other possible gradients. Single-fluid models have the advantages of being formulated from physically intuitive arguments and yielding relatively simpler transport equations. Such equations may be useful for describing steady-state flow, but are not likely to be useful in situations where the flows are quite different for each component (e.g., transient flows).

A second class of phenomenological approaches treats the fluid and solids as two separate phases, with the solid also treated as a continuum phase. In these models, the motion of each phase is described separately, but in order to complete the equations, one needs to develop constitutive relations, and the development of physically intuitive (or physically reasonable) relations is a weak link. For example, the solid phase is generally assigned a "viscosity" independent of the presence of the liquid, and the meaning of this "viscosity" is uncertain and may not be related to measurable quantities. Moreover, cross-terms that address solid-liquid lnteractions are difficult to derive and relate to physically meaningful processes. A variation of these two-phase approaches has been developed using "averaging theory" concepts that have been applied with some success to gas-solid flows. In _, these averaging theory approaches, the governing equations are derived by summing up, equations for small, single phase domains. The result is that the critical information required to describe the flow is concentrated in integrals which represent the interactions between the solids and liquid. Evaluating the integrals in terms of basic physical mechanisms is highly complex, and further research is required to determine whether this approach will yield physical insights regarding how the formulation of a suspension determines its flow properties.

Kinetic Theories:

Kinetic theory has been successful in obtaining governing equations and transport coefficients for gases. Recently, kinetic theories have been extended and used to study the flow of granular materials. Success in this area appears to be based upon the similarities between random molecular motions in gases and the fluctuating granular motions within granular flows. In kinetic theories, the system is described using distribution functions for the location and velocity of the solid components. Interactions are modelled in terms of collisions. In flows of heavily-loaded suspensions, interactions between solid particles are inherently hydrodynamic and cannot be described as isolated two particle events. Thus, for the same reasons that kinetic theories are not useful for describing the behavior of liquids, kinetic theories are unlikely to be useful in developing the transport equations for heavily-loaded suspensions. However, some techniques from kinetic theories may be productive in developing physical insights.

Statistical Mechanics:

Statistical mechanics herein refers to methods that derive microscopic field equations starting from the equations of motion of all of the constituent particles. Properly applied, statistical mechanics is rigorous in the sense that a physical meaning can be attached to all assumptions. The main value of statistical mechanics with regard to suspensions is that this approach can shed light on the fundamental form of the governing equations and relate the various terms to underlying physical mechanisms.A recent example of the successful application of statistical mechanics is the use of mode-mode coupling theories to derive nonlinear hydrodynamic equations that can recover the Navier-Stokes equations for simple fluids and identify the correction terms. With regard to suspension flows, only limited research has been accomplished. For example, for N large particles submerged in a bath of small particles, a Fokker-Planec equation has been derived for the near-equilibrium distribution function. With additional work, it should be possible to establish the generalized forms of the governing equations. However, considerable research would be required to reduce this generalized form to a tractable set of equations.

B. Transport Coefficients

Once proper forms of the governing equations are available, it is highly desirable to have a theoretical basis by which the transport coefficiencies can be predicted from a knowledge of the composition of the suspension. For example, the study of the apparent viscosity of suspensions is an important topic. It is known that this transport coefficient depends not only upon the concentration of solid particles, but also upon the distribution of particle sizes. In addition, there may be an important contribution from the shapes of the solid particles. Moreover, particle-particle and particle-liquid interactions are quite different as particle sizes move from the submicron range to the 100 micron range. For the former, colloidal effects predominate, whereas for larger particles, hydrodynamic interactions become important. The study of colloidal systems is a large field, and while progress is being made, it is unlikely that major advances in colloidal transport will occur during the next few years. However, it should be possible to decouple, to some extent at least, the problem of heavily-loaded suspensions from the very complex problem of predicting the transport behavior of colloidal systems as well as the impact of surfactants and additives on the transport properties of colloidal systems. For the near-term, the most productive theoretical approaches will perforce rely upon phenomenological concepts. Using statistical mechanics, some progress has already been achieved in deriving expressions for the viscosity of a suspension of large solid particles in a Newtonian liquid. Further work in this area may also be productive.

C. Theory Verification

Selection of preferred theoretical models requires a comparison of theoretical prediction with experiment. In this area, the goal is to concentrate to the extent possible on geometries and experimental conditions that isolate particular flow effects. For such relatively simple conditions, solution of various proposed transport equations for different boundary conditions is still a challenging problem. Normally, these equations are solved numerically, and this subject is discussed below.

II. Experimental work:

(1) reveal structural information such as particle migration (shear thinning), particle clustering, etc., that will help to understand the underlying physics.
(2) determine transport coefficients and establish fundamentals regarding constitutive relations.
(3) verify the theoretical calculations in predicting the pressure loss in flow fields.

(4) test realistic situations such as the flow of suspensions in pipes, convergent and divergent
(5) sections, bends, and simple flow splitters (e.g., wedges).

The key variables to be measured are concentration and velocity distributions as a function of spatial coordinates and time, and the fluctuations of these variables. Since we are interested in the evolution of non-homogeneities, the concentration distribution is an important quantity to measure. The distributions of velocity and concentration are the essential ingredients for calculating stress information needed to get pressure loss over a distance and the friction forces on walls. The time evolution is important to see whether there is a steady state and how long it takes to establish. Fluctuations give us a measure of the deviation from mean values. Suspension flow appears to be laminar for high concentrations, but the motion can be turbulent when solids concentrations are moderate. For the case of small fluctuations, the mean values give a good description of the system, but for flow with large fluctuations such as turbulence, the knowledge of mean values is not enough. Fluctuations in velocity will also give rise to an additional stress, the Reynolds stress.

Possible measurement tools include optical, NMR (Nuclear Magnetic Resonance) and acoustic methods. NMR imaging can provide both concentration and velocity profiles of suspension flow. For the measurement of solid-liquid flow, NMR is a relatively young technique and holds great promise. The disadvantage of this method is that the time response is relatively long so it is unlikely to be useful for measuring fluctuations.

Optical methods have been used in the measurement of fluid mechanics and dilute solid-liquid flow. With the help of tracking particles, optical imaging can measure velocity and concentration profiles. Laser Speckle Velocimetry can be used to determine r.m.s. velocities. Laser Doppler Velocimetry can make rapid measurements of local velocity and can give both the mean velocity and its fluctuations. The advantages of optical methods are their fast time response and fine spatial resolution and some of them can provide temporal and spatial fluctuations in addition to the mean value measurement. The shortcoming is that they are limited to systems in which the refractive index of the solid particles is matched to that of the fluid. In general, optical methods are ideal tools in the measurement of model systems.

Acoustic methods are also capable of determining concentrations. By using the Doppler effect, they may also give velocity information. The major disadvantage of acoustic methods is that the spatial resolution is limited by the sound wavelength. The advantage is that they are usually less expensive and more robust than optional methods. They may be ideal tools for monitoring and diagnostic purposes in industrial sites.

Experimental work is also required in the study of constitutive relations and transport coefficients. Experiment can verify theoretical predictions and provide a basis for deriving empirical formulas. These investigations are especially important because most theoretical approaches are phenomenological and need to be verified carefully. Special attention should also be paid to the accuracy and measuring techniques because of the time dependent nature of suspension flow. An important area for experimental work is in measuring the apparent viscosity as a function of the solids concentration, size, and shape distribution, as well as the dependence of viscosity on surface treatments. Dynamical measurements are also needed to determine the pressure loss and the friction forces on walls.

III. Numerical Methods

The rapid development of computer technology and numerical calculation methods provides another important tool in the study of this complex system. Since the continuum equations involved here are nonlinear, numerical solutions of the field equations are required. We would not be able to check different theoretical approaches unless we can compare the results of the calculation based on these approaches for different geometries. In this regard, the numerical solution of various governing equations under different boundary conditions is an inseparable issue and should be closely related to theoretical studies.

The numerical solutions may be required in determining the transport coefficients. For example, the apparent viscosity may be numerically determined by calculating the forces on N particles submerged in a fluid. Computers can also be used to simulate the motion of the suspended particles. However, it is not an easy task to simulate a great number of particles in a fluid. Recent developments in simulation techniques (such as cellular automata) have used lattice gas models to simulate the motion of liquids. This work provides a method to carry a molecular-dynamics type approach to simulate the motion of suspended particles. The simulation of a suspension is a challenging task, but it has the potential to give very useful information if successful. Such computer simulations are numerical experiments that may give information that is difficult to measure in real experiments. Moreover, they allow the researcher to isolate the effect of each parameter.

RECOMMENDATIONS

This program is expected to last seven years. For the first three to four years of effort, the following research efforts are recommended.

I. Establish preferred phenomenological approaches. It is possible that more than a single approach may be required, depending on the flow regimes and suspension formulations.

(1) Refine the derivation of various phenomenological approaches.
(2) Resolve disparities between various approaches.
(3) Experimental (and some numerical) discrimination of various approaches.

II. Devote a small effort in the derivation of general forms of transport equations using statistical mechanics. Such effort is important because the approaches are more rigorous and may provide some guidelines.

III. In the study of transport coefficients, primary efforts should be devoted in phenomenological and experimental study with a small amount of effort in pursuing statistical mechanics approaches and computational study of transport coefficients (e.g., calculating forces of a large but finite number of particles submerged in a fluid).

IV. Important quantities to be measured in the experimental study are transport coefficients and flow fields (concentration and velocity distributions as a function of space and time). In the first three years, major efforts should be focused on optical and NMR methods.

(1) Optical methods including imaging, LDV, tracking particles and speckle spectrum can be used to measure the velocity and concentration distributions and fluctuations.
(2) NMR is useful to measure the concentration and velocity distributions. This method is especially important for highly concentrated flows.

Purpose: To develop a consistent set of concentrated slurry conservation equations and best-estimate constitutive relations. To demonstrate the feasibility of experimental techniques in validating both the conservation equations and the constitutive relations.

WORK SCOPE/BRIEF PROJECT SUMMARY:
The two components of the proposed research supporting the major long-range initiative (see Background) are divided into theoretical and experimental activities.

Theoretical
A new integral control volume formulation of the conservation equations based on particle motion will be developed. This new formulation differs with others and it provides direct linkage between microscale solids motion and interactions (solids-solids, solids-fluid) and macro-characterization of concentrated solids suspensions. The relative importance of stresses, fluxes, and forces acting on particles will be evaluated utilizing the proposed formulation and experimental measurements. Limited numerical analyses will be performed to quantify various contributions in the conservation equation for the concentrated slurries.

Experimental
Recent emerging state-of-the-art experimental techniques involving flow visualization particle image tracking will be further developed and shown to be capable of measuring the discrete microscale data needed in the long-range initiative. To date there is no published information of the data needed for this initiative. Specifically advanced video-optical/digital laser sheet imaging will be used with index of refraction matching between liquid and particles for the study of the highly-loaded micron sized particle slurries. Instantaneous local fluid and particle velocity (mean and fluctuation) along with temporal phase information will be shown to be capable of measurement in a proof-of-concept test. This unique information is needed to evaluate various stresses, fluxes, and forces in the control-volume formulation of the conservation equations.

BACKGROUND: The long-range plan seeks to develop a self-consistent methodology to link micro-and macro-fluid mechanical phenomena associated with slurry pipe component flows. This approach will gain fundamental understanding and enable sound design and safe operation of slurry piping systems.

The long-range plan is comprised of the following two phases:

Phase I:
Theoretical: Investigate and systematically evaluate various theoretical governing equations and constitutive relations including transport coefficients.

Experimental: Establish a capability and operate an experimental facility at ANL for the use, improvement, and development of appropriate measurement techniques for the study of suspensions and provide data necessary for model validation. This activity would also serve to integrate and evaluate those techniques developed by other researchers and apply them in making fundamental microscale/macroscale measurements. Tests with particular emphasis on particle-particle interactions mediated by interstitial fluid will also be conducted.

Engineering Analysis: Perform engineering and numerical analyses to evaluate various formulations and related experimental data. ANL will create a library for archiving and disseminating the experimental data generated in the program.

Phase II:
Validate constitutive relations and transport coefficients models for complex piping system components comprising elbows and flow splitters, and investigate and extend the range of applicability as necessary. Conduct piping component flow experiments to furnish data for model and code validation. Develop an engineering handbook and appropriate supporting items, such as an engineering analysis code, for the formulation of heavily loaded suspensions, the prediction of suspension flow behavior, and the design and scale-up of suspension piping systems. Develop the necessary materials to facilitate technology transfer.

JUSTIFICATION: The DOE (Fossil Energy) has identified a need for long range research on concentrated suspensions (slurries). The program as envisioned by DOE would be nominally of seven years duration and be funded in the order of 2 million dollars per year. Unfortunately, it will take a year or two before DOE will be in a position to consider funding this effort, the LORD will be used to prepare a strong technical argument that such a program is feasible.

In addition, a RAND Corporation study has found that there is a large class of industries that process solid materials that have performed poorly and little progress has been made in improving their performance. More specifically, many problems have centered around coal/liquid suspension flows in piping as related to coal preparation, liquefaction, and combustion systems. Currently there is little reliable information for predicting flow behavior in simple components (i.e., bends, splitters, and straight runs) which comprise a pipe system. This long-range initiative would provide fundamental understanding and guidance to the industry for properly designed concentrated slurry systems.

C. Questions and Answers Posed in my Presentation at the 2010 Workshop on Multiphase Flow Science [24]

1. Are the three Transport Gasifier-scale metrics/benchmark cases realistic? **These are realistic, but not quantifiable and thus do not meet the need of providing demonstrated utility. These benchmarks address the issues of processing speed, development of fast algorithms, and incorporation of complex chemistry and fluid dynamics. There is insufficient data available from the benchmark experimental units to provide objective and quantifiable criteria. None of that data has been presented to the MF community. As such the Additional cases are required to address the accuracy and reliability of the codes. It is these latter cases which are needed to understand and document where different codes succeed and what are their limitations. A first step is to use the Challenge Problem posted on the NETL web site to evaluate fluidized bed and circulating fluid bed hydrodynamics. In the future, a benchmark case directed at carbon dioxide capture with solids sorbents would represent more relevant research goals consistent with funding sources, with simpler and more quantifiable chemistry.**
2. Should other metrics be added? **YES**—What do you propose? **See #1**
3. What technology gaps are missing? **Measuring Granular Temperature, gas solids viscosity, Boundary conditions**
4. Should all submodels be analyzed using MFIX? **A series of defining standards should be established to verify submodel and quantify submodel robustness and accuracy.**
5. Should chaos, slurry, and particle rotation and attrition be added? **This depends on the target desired application—current no vision is defined which considers and focuses efforts on the most critical applications. This vision should be no less than 3 years out and no more than 5 years. CO_2 capture is a relevant primary DOE vision—if that focus leads to entrained gasifiers then slurry is important, transport gasifiers look at chaos and rotation, FB CO_2 sorbents look at chaos, and all three need attrition mechanisms.**
6. What equations are best to use for simulations? **Funding these areas may be needed to define that.**
7. Should DEM be compared with Eulerian-Eulerian, and/or Kinetic Theory? - When - Why - What applications? **To my knowledge there is still a need to defining expressions for heat transfer as well as wall surface boundary conditions. DEM seems more appropriately applied to determine boundary conditions for wall interactions, effects of size and shape, roughness, granular temperature effects, chaos influences.**
8. What simple, well-defined experiments are missing? **Experiments with multiple diagnostics defining particle and gas mixing and residence time distributions - these are measurements needed to obtain reasonable reaction performance to validate process reactions**

9. Is enough emphasis placed on sub-models for reacting systems? **NO**
10. Has the roadmap gone far enough and should the time line be extended? **Extended**

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Notes

Dedication

The photo of Professor Dimitri is by Renee Mercuri (Reprinted with permission. Copyright 2007 IIT). Beisel, C. L., Faculty Achievements. *Crosslinks, the Newsletter of the IIT Department of Chemical and Biological Engineering,* Fall 2007:10 (2007).

The photo of Charles W. Solbrig was sent to me by him.

Chapter 1

Page 2 "This book rights the slights of Stan Fabic's brief survey of best-estimate codes funded by the NRC [7]…" After my manuscript was basically completed, Dan Hughes alerted me to the fact that Stan Fabic had published his memoirs [1]. In the Chapter **Life In Maryland (1973-)** he gives an extremely terse account of his role, when he worked for L. S. Tong at the NRC, in dismantling the computer code work which was ongoing at INEL without mentioning a single name or code. His stated rational was that he "…had to redirect focus to LASL because of its expertise in applied numerical analyses, the area in which INEL appeared weak."

1. Fabic, S., *My Life on Three Continents*, Xlibris Corporation (2012).

Chapter 3

Page 24 "While at ARF/IITRI Charlie did research on a turbine compressor, a multifuel diesel engine, a smokeless oil burner, thermal radiation, and measurement of explosion limits in space simulation chambers [5]."

Charlie did many projects at ARF including testing the radiation output of aircraft decoys which were to attack the missile rather than the plane. Another was investigation of explosion limits of vacuum diffusion pump oils. It was at low pressure but somehow over the night an explosion occurred and a high vacuum pressure gauge shot up and put a dent in a 20-foot-high ceiling. He never saw any explosions in any of the testing. So he figured analytical work was safer although he has done other experimental work since then.

Page 25 "Charlie took the three-day written comprehensive examination with two other Ph.D. candidates who had taken a year to study for it. One was asked to leave the program and one did so well that he was able to skip the oral exam."

R.W. Lyczkowski, *The History of Multiphase Science and Computational Fluid Dynamics*, Mechanical Engineering Series,
https://doi.org/10.1007/978-3-319-66502-3

It was Elwood Roth who was asked to leave. No one saw him after the exam. He disappeared. Joseph Dolan was the other and he did so well on the written he did not have to take the final. He died quite young.

Page 25 “This was to be a purely analytical study because of Charlie’s experience in the IGT Fluid Properties Laboratory, which had to be evacuated because of an accident whereby mercury liquid and vapor were released from an extremely high-pressure apparatus thereby contaminating the laboratory. Charlie entered the laboratory to shut off the leaking pipe thus exposing himself to the mercury vapor.”

Charlie was working at a desk in the lab. Bill Reppin was transferring mercury from one high-pressure vessel to another with a high-pressure gas-bottle attached to the top of one vessel and connected by a line on the bottom to another vessel. Bill was a heavy smoker and was walking around not paying attention since it was a slow process. The one vessel emptied and gas started bubbling thru the other vessel and spraying miniscule particles of mercury over the whole room. Everyone evacuated the room including Charlie. However, he ran back in and closed the valve in the line between the vessels to stop the spraying.

Page 25 “Charlie was ensconced in the basement, separate from all the other students in an office which he shared with a defunct, non-operating electron microscope.”

He and Dimitri shared the electron microscope office when he returned to graduate school for his Ph.D. He was in the six-person room in the basement as a Masters student with Ken Starling, Dan Magasanick, Joe Dolan, and he thinks Frank Kulacki. Dimitri got an office on the top floor and so moved up there. The electron microscope room was right next to the computer room. Charlie was always in there compiling programs. The IBM 1620 had a paper-tape drive because Dr. Weil was afraid people would drop the deck of cards. It took 45 minutes to compile a program. One mistake, another 45 minutes.

Chapter 4

Page 40 “Some are described in “The 'Calculated' Loss-of-Coolant Accident–A Review” [4].”

It is important to note that Charlie reviewed all the vendors’ blowdown codes and knew all the defects of these codes which allowed him to write this review. Neither Larry nor Isbin contributed much to it. Charlie was a consultant to the ACRS and went to all their sessions where he (and other consultants) and committee members questioned the endors about their license applications.

Chapter 5

Page 54 “One of the more interesting ones was reviewing alternative processes to separate uranium isotopes such as shock waves in the Becker nozzle…”

Becker, E. W., K. Bier, W. Bier, R. Schutte, and D. Seidel, *Separation of the Isotopes of Uranium by the Separation Nozzle Process*, Angew. Chem. Internat . Edit., Vol. 6, No. 6:507–518 (1967).

Chapter 6

Page 75 "We were able to document in a paper prepared for the November 1973 American Nuclear Society Winter Meeting (but never submitted for publication) that imaginary characteristics can result even for the two cases of equal phase velocities and zero relative velocity."

This paper was incorporated into the published version of the characteristics paper reference [15] in Chapter 8 where these equations are given.

Chapter 7

Page 114 "He remembers that during his presentation for the SCORE code as he showed the slide for the volume averaged equations being solved and he said…"

Notwithstanding the minutes of the meeting, Dan cannot recall with certainty that he was presenting the SCORE code. He thinks he would not have said, "We solve the three dimensional Navier-Stokes equations", if he was in fact presenting the SCORE code equations which have embedded solids represented via volume averaging. His statement is more consistent with the initial SPLEN code, using Reynolds Averaged Navier-Stokes (RANS) model. Whatever the case, the volume-averaging approach, as we know well, is universally accepted. For a discussion of volume averaging the reader is referred to Hughes [1] and to Ishii and Hibicki [2].

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Chapter 8

Page 131 2nd paragraph Because of Stadedke's outright dismissal of two-pressure two-phase models in his book, this caused me to re-examine my collection of literature on the modeling of stratified flow. I found that the two-pressure model by Robert R. Long, *Long Waves In a Two-Fluid System*, Journal of Meterology, Volume 13:74 (Feb. 1956) contained the earliest reference to the fact that the characteristics are not necessarily real!

Chapter 9

Page 140 "The code solves the one-dimensional HEMM model describing steady and transient one-component…"

RETRAN has a five-equation model. The user can choose three, four, or five equations. It has a six-equation model for specific components and regions of plants. It can be coupled to three-dimensional neutronics.

Page 140 "RETRAN is a state-of-the-art computer code developed primarily for licensing and safety analyses for the electric utilities' nuclear power plants. It is designed to analyze a wide variety of fluid flow and heat transfer problems for complete nuclear and fossil power plant systems."

RETRAN went on to become a success in the utility industry. The code began to be widely adapted by the US utility industry shortly after its approval by the NRC in 1981 for applications to operational and safety analyses. Within that industry, and other national and international organizations, RETRAN remains successful to the present day.

Chapter 10

Page 150 "When He returned to EG&G, Idaho Inc. in 1980 he became Manager of the LOFT Program Division."

Charlie was in Chicago working for Commonwealth Edison as their Nuclear Safety Expert in 1979. Nick Kaufman replaced Larry as Manager of the LOFT Division. Nick Kaufman called Charlie in Chicago and asked him to take the job of LOFT Analysis Division Manager. which he did. LOFT had four divisions of which he managed one on them.

Page 154 "He noted that it would be difficult to license a nuclear power plant without using the data from the INL tests and RELAP5."

When Charlie left the SLOOP code group in 1975, he went into the experimental side of two-phase flow. Initially he ran and set up testing for the two-phase instruments developed for LOFT. In 1980, he was called back to plan and organize the LOFT nuclear large and small break LOCAs and anticipated transients. These along with Semiscale are the tests Myer referred to as necessary for today's licensing of nuclear reactors.

Chapter 16

Page 217 "The purpose of this task was to document industrial case studies of a non-proprietary nature that would clearly demonstrate the ROI of CFD modeling which would help the DOE OIT to justify present and future funding of the MFDRC…"

The following was my proposal for this task.

Determination of the Return Of Investment for CFD Modeling

The strategy for determining the return on investment for computational fluid dynamics (CFD) consists of quantifying the savings produced by several components. These quantitative components include: 1.) reduced time to finalize a design change to mitigate a specific problem, 2.). reduction in the number of laboratory experiments to test the design change, 3.) reduced time to scale up by reducing the number of pilot plant stages, 4.) elimination of large scale experimental facilities, 5.) decreased plant down-times. 6.) increased throughput, 7.) process optimization for improved energy efficiency, 8.) reduction in pollutant formation, and 9.) streamlining the supply chain. Putting numbers on one or more of these components will be the thrust of this project. It should be emphasized that there are, in addition, qualitative benefits associated with CFD modeling such as better understanding of process behavior and increased ability to innovate.

The general perception is that the return on investment (ROI) of multiphase computational fluid dynamics (CFD) modeling in the chemical industry is significant. Industrial leaders in CFD modeling (primarily single phase) are Dow Chemical and DuPont with up to nearly two decades of experience apiece. Firstly, one can speak in terms of broad generalities about multiphase ROI based upon the following facts and findings. At least 40% of all chemical processing in the United States involves handling solids, from the introduction of raw material to the packaging of the final products. While chemical plants that handle liquids and gases enjoy an average efficiency of approximately 84%, producers handling solids experience a disappointing 63% efficiency [1]. The poor efficiency is largely attributed to limited, fundamental understanding of the dynamic behavior of gas-solids flows and the consequent lack of design tools based on that fundamental understanding. Domestic chemicals companies linked to particle technology produce more than $61 billion/yr [2]. These studies do not address the efficacy of multiphase CFD modeling. We can conservatively estimate that if CFD modeling could produce only a one percent narrowing of the gap of the difference in efficiencies between liquids/gases (84% efficiency) and solids/liquid/gases (63% efficiency) this would result in a $200 million/year savings for US chemical industries. Correspondingly, a 5% improvement would mean a savings of one billion dollars/year. The missing parameter in this equation which hinders the determination of ROI is how much needs to be spent to effect these savings, $1,000,000, $10,000,00/year, more? This is the parameter this project seeks to determine.

The benefits of using CFD modeling in general to enable process improvement are commonly discussed within the scientific community. Many companies have shared their experiences in open forms; such as, the “Reaction Engineering and Computational Fluid Dynamic Form”, held by The Engineering Foundation in San Diego, CA (1996). It is also shared in semi-open form through the Chemical Producers Computational Fluid Dynamics User Group (CPCFD). Presentation for the last several meetings may be found on the Internet at: www.cray.com/cpcfd. As willing as the CFD community is to agree on the usefulness of the tool, companies are very guarded to share any dollar amounts saved from direct insight gained from using CFD simulations because of the highly competitive nature of the industry.

There is some global data made available from the world’s largest CFD software company, Fluent, Inc. The average annual benefit to cost ratio, i.e. the average value added to the company’s operations compared to the cost of CFD software, for the average company licensing Fluent, Inc. software over a five-year period is in the range of 5:1. This value is based on Fluent, Inc’s experience in marketing CFD software over a number of years. This is only one component in the ROI equation.

The purpose of this project is to document industrial case studies of a non-proprietary nature that will clearly demonstrate the return on investment of CFD modeling This will help the DOE OIT justify present and future funding of the MFDRC in particular and multiphase CFD in general. In addition it will benefit the awardees of proposed projects. The return should not only include the cost of the software, but also the engineer’s time to set up the problem, perform the computations, analyze the results, and generate cost savings and/or productivity gains based on insights generated. A large addition to the ROI accrues if a pilot plant step or large scale experimental facilities can be eliminated and/or reduced.

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Chapter 20

Page 236 "Another instance of the politics of science was Frank Harlow's copying Charlie's equations which lead to the development of the KACHINA, K-FIX and TRAC computer codes at LASL."

Today one would call this "research misconduct" or a breach of research ethics. It might justifiably be called plagerism.

Page 237 "Following the tragic Piper Alpha incident…"

Piper Alpha was an oil production platform in the North Sea approximately 190 km north-east of Aberdeen, Scotland, that was operated by Occidental Petroleum (Caledonia) Limited. An explosion and resulting oil and gas fires destroyed Piper Alpha on 6 July 1988, killing 167 people, including two crewmen of a rescue vessel; 61 workers aboard survived. Thirty bodies were never recovered. The total insured loss was about £1.7 billion ($3.4 billion), making it one of the costliest manmade catastrophes ever.

Appendix J

This appendix is a reformatted and corrected version of the original report sent to NETL and is contained here with Dr. Madhava Syamlal's permission.

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https://doi.org/10.1007/978-3-319-66502-3