CAPE Role in Engineering Innovation: Part 1-The evolution

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Abstract. The advancement of science in the past century gave rise to a number of revolutionary discoveries that deeply affected the way of life of our society. Here, is given a personal summary of the variety of applications evolving from a major discovery, the analytical engine, which instrumented a novel, revolutionary *software engineering*, enhancing the now so called Computer Aided Process Engineering in a variety of applications. The race among software-hardware has made possible fast pace in the *evolution/revolution* that affects all branches of science towards new discoveries with different impact and magnitude. The reader is guided on a tour through various milestones lived, whose main protagonist is an increasingly sophisticated software. Applications to a variety of *systems*, like telecommunications, biology, chemical engineering, mechanics, mining, etc. are revisited.

Keywords: Software Engineering, Computer aided process engineering, Process systems engineering.

1 Introduction

It has been fascinating to observe the advances made by science in the last century. We witnessed an incredible number of discoveries that changed our lifestyles, affected our society and had a profound effect on deeply held beliefs. Some of these discoveries were *revolutionary*. Television, atomic energy and satellite communications form part of a list of inventions too long to mention in full [1].

One significant discovery was the *difference engine*, which could be said to be the first computer. It was the computer pioneer Charles Babbage (1791-1871) who devised two classes of engines, the difference engine and the *analytical engine* [2]. This last one gave place to fully-fledged general-purpose computation leading to the now so called Computer Aided Process Engineering in a variety of applications. This *revolutionary* computing invention opened new doors and perspectives, mainly because it offered solutions to problems that had for a long time remained unsolved.

Let's go on to *describe some examples* that I have come across in my personal experience of CAPE's role in the evolution of engineering.

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2 Samples of the past

2.1 Modeling Telecommunication Systems

When I became part of NASA Aerospace Telecommunications Unit in 1965, the avalanche of great discoveries that surrounded us was fascinating. In my case, my quest was to find a way of conveying a huge number of signals with a minimum loss of power. Multiplexing systems (Fig. 1) already existed, but inter-channel crosstalk was a major problem in manned space flights. On these flights, trajectory and telemetry data, which provide both positional and environmental parameters about the spacecraft and the astronauts, must be processed immediately upon their arrival by a real-time operation system via a worldwide communications network. A new framework for a fast and reliable telecommunications system in real time was needed.

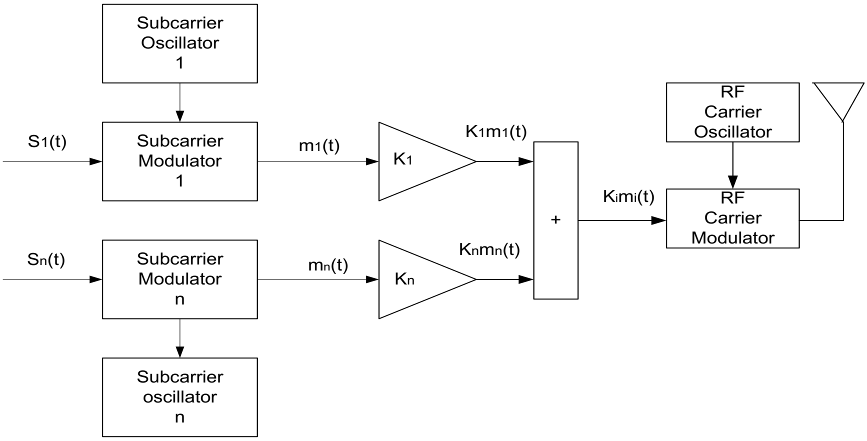
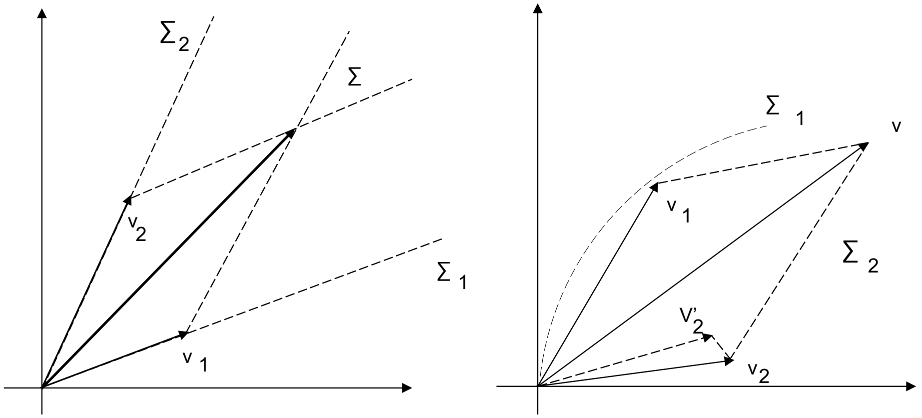


Fig. 1. Multiplexing System SSC-FM block diagram

The model proposed uses a novel analytical signal representation for the real signal. Its advantage is that the phase and envelope of the real signal can be fully described and represented in the upper half of the complex plane. Moreover, the phase and envelope are actually given in terms of the zeros of the analytical signal: the so-called "zero-locus" [3].

The phase or envelope can be manipulated to produce different signals that do not interfere with one another. Thus, a "common envelope set" will be obtained that contains signals that differ in phase but not in envelope or bandwidth. Computationally speaking, this means that one may easily track the real modulating signal through the zeroes of its analytical signal in the complex Z-plane.



Geometrical representation for linear signal-space

Effects of distortion in signal-space representation

Fig. 2. Crosstalk effects of distortion in signal-space representation

The zero representation was used to study various forms of modulated waves. This representation was based on the principle of factorization in terms of the Fourier series expansion, and on the property of zero-pattern superposition that results from the product of two or more signals. Multiplicative processes are the most amenable to a zero-based description. Special attention was also paid in the study of crosstalk effects, Fig. 2 [4]. Tensor analysis was employed in the multi-space in which the zeroes of multiplicative signals are located. The evaluation of crosstalk in terms of tensor forms resulted in an advantageous simplification in the calculation procedure.

I consider that the use of CAPE in this case constituted real innovation in a field lacking mathematical models. I would even go as far as to say that this advance is particularly significant as it still applies today.

2.2 The Stochastic Computer

The *next example* illustrates CAPE's ability to introduce new concepts in computing techniques. As a departure from conventional digital or analog computing technologies, the stochastic (random-pulse) computer utilizes logical elements (gates) to process the analog magnitude that has been chosen to represent the variables (Fig. 3). The aforementioned analog magnitude is the probability of pulse-occurrence in a train of random pulses [5]. The variable value is recovered by averaging the stochastically coded variable over a period of time that is assumed to be stationary. It is readily apparent, for instance, that given that two statistically independent stationary random-pulse trains drive the two inputs of an AND gate, once the output pulse train is eventually reshaped it will have a probability of occurrence equal to the product of the probabilities of the incoming inputs [6]. A straightforward multiplier is thus obtained.

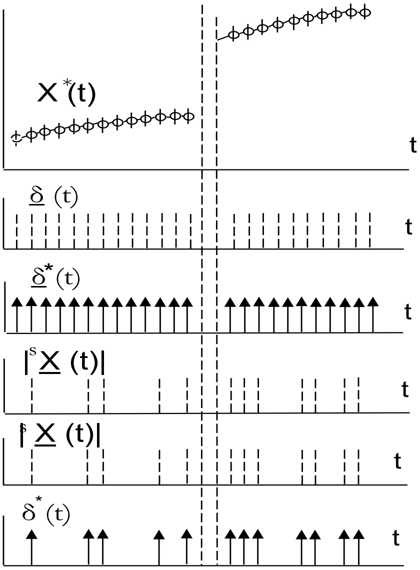


Fig. 3. Stochastic representation of variables

A random floating point stochastic coding was proposed through the use of weighted probabilities in order to increase the dynamic range of the variables to values of less than 1. The implementation of generalized (random floating point) stochastic coding made it possible to generate arithmetic operators (addition and subtraction) in a straightforward fashion, as well as to come up with the product and quotient. Integration and derivation can be easily performed by means of a bidirectional counter with weighed inputs followed by a digital to stochastic converter.

In order to generate functions in stochastic computation, a highly stimulating method that is *unique* to this technology was envisaged. In the case of linear stochastic conversion, the random-pulse train is a true stochastic representation of variables. However, this requires a uniform probability density function. This means that white Gaussian sequences, which were very difficult to obtain, must be used.

Alternatively, if at the stochastic conversion stage the cumulative probability function of a sampled random noise is not linear, but is instead an arbitrary monotone increasing function, the encoded variable would be the stochastic representation of this function, which is thus directly obtained. [7].

The problem of function generation is related to the problem of generating functional noises with specified cumulative probability functions. Pseudo-random *dinary* pulse-trains were proposed instead of random binary pulse-trains. This noise can be easily generated using the technique of maximum-length sequences, which is attained through the use of shift registers with appropriate feedback paths. The physical implementation was a module 127, three-stage shift register, which directly generates a maximum length sequence of 127^3-1 numbers of seven digits (equivalent to 127 levels) thus giving a computing accuracy of 0,1.

I consider multichannel stochastic computation to be *a wholly innovative concept* with practical evidence in control applications. Traffic control is a major application of this technique. Strangely enough, the whole traffic control project was licensed to the Russians. Ironically, it was to be implemented in Moscow in 1969, which at that time had a very low traffic density.

2.3 Modeling Macromolecules

My next example is closely connected with the extraordinary experience of working with two Nobel Prize winners, Maurice Wilkins and Jean Hanson, at King's College, London. Maurice Wilkins, a brilliant physicist, continued his excellent work on the *X-ray fiber diffraction of macromolecules*. In 1966, he and his PhD student, John Pardon, invented the toroidal camera, which made it possible to obtain precise, low-angle diffraction patterns that gave an accurate picture of long-pitch helical molecules such as nucleohistones. The remaining problem was to *find accurate structural models of complex macromolecules*, which led to a *refined tertiary structure of biopolymers*.

The advances in computer power and satellite technology were enthusiastically adopted by leading biophysicists around the world. I then worked with Wilkins at King's College and went on to work with Struther Arnott at Purdue University on DNA forms and complexes Fig. 4.

Fig. 4. B-DNA X-ray fiber diffraction pattern

A working model and strategy to overcome these issues were once again necessary. Arnott (an ex–fellow of King's College) and Peter Campbell came up with the most successful strategy for modeling and refining macromolecular structures [8]. As a result they created the core of the *linked-atom-least-squares* program (LALS), which was subsequently improved by several others, *myself included*.

The basic repeating structure – the nucleotide residue – was established by defining six conformational angles with which to build the anti-parallel chains and the glycosidic angle that linked them to the sugar rings. Five additional degrees of freedom made it possible to move the configuration of sugar to C'2 endo and C'3 endo puckering [9].

As part of my work involved in the *prediction of a rich variety of DNA configurations*, intensities along the different layers of this reciprocal space were mathematically calculated. This was done by taking the inverse of the Fourier transform, which was approximated by Bessel functions in the reciprocal space. As a final outcome, the radius and position, or phase, of each molecule's atom was obtained. The *model optimization* – the refined molecule structure – was obtained by minimizing the difference in structure amplitudes subject to the relative weight of the observations. Stereochemical acceptability was ensured by taking into account the interatomic distances d_j, which was calculated using a Buckingham energy function.

It was extremely rewarding to see that the *predicted variability did indeed correspond to physical structures* [10]. The two "classical" forms of DNA – A and B – gave rise to a variety of intermediate structures, which coincided with the actual binding of proteins (Table 1).

The comment "*a small step for mankind, but a giant step for Luis*" were dedicated to me by Struther Arnott when, by chance, I discovered *heteronomous DNA*, popularly called Z-DNA [11]. This discovery was related to the puckering of the sugar rings that changed from one nucleotide to the next. This caused real "kinks" in the structure that resulted in a superhelical structure, which had been theoretically predicted in the case of nucleohistones.

The Z-DNA fragments may constitute the building blocks that are embedded in the classical A and B forms of DNA, which give rise to hybrid structures. This *revolutionary* vision of DNA was reached rapidly, largely thanks to the advances made in computing power. Instead of the IBM 7094 with 170 kB that had been used in the past, the 8MB Cray supercomputer was developed. This development was superseded by the Cray Y-MP in 1988, which performed at a speed of 1Gflop. However, the enormous importance attached to this research subject also meant that the consolidation of CAPE tools relied heavily on contributions from other disciplines, such as quantum chemistry, which is the case today.

Table 1 DNA variety and variability

Family	**Furanose Conformations**	**Conformational Genera**	**Number of Congeneric Species**	**Helical Characteristics**	
				h(nm)	**t(°)**
A	C3' - endo	$t\ g^-\ g^-\ t\ g^+\ g^+\ a$	16	0.26-0.33	30.0-32.7
		$t\ g^-\ t\ t\ t\ g^+\ a$	1	0.31	36
B	C2' - endo	$t\ t\ g^-\ t\ g^+\ t\ a$	4	0.30-0.34	36.0-45.0
		t t t t t t a	1	0.33	48

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2.4 Modeling Fluidized-Bed Reactors

Modeling fluidized beds was complex enough, but coupled with the study of gasification reactions, the system was doubly complicated. Levenspiel (in 1976) encouraged me to *embark on a still more complex journey*: to trap the bubbles that deteriorated the fluidized bed's performance using a magnetic field [12].

A model already plagued with empirical correlations would not dare to reject meta-models that were based on laboratory experiments! Although the appearance of fluidization curves was similar for fluidization with and without a magnetic field, two important phenomena were observed. On the one hand, bench scale experimentation demonstrated that a "calming" zone could be reached within a certain range of magnetic field intensity. Within this range, the fluidized bed becomes stabilized and by-passing bubbles of the gas carrier vanish.

If the magnetic field was switched off, bubbling increased and turbulence was much greater. The gas limit velocity at which bed expansion was obtained without turbulence was named the "transition velocity u_b", after which bubbles would dilute (Fig. 5). The transition velocity could take values up to eight times the minimum fluidization velocity. It can be predicted as a function of the bed porosity, the angle of mean velocity u in channels and vertical axis, and the magnetic field intensity H [13].

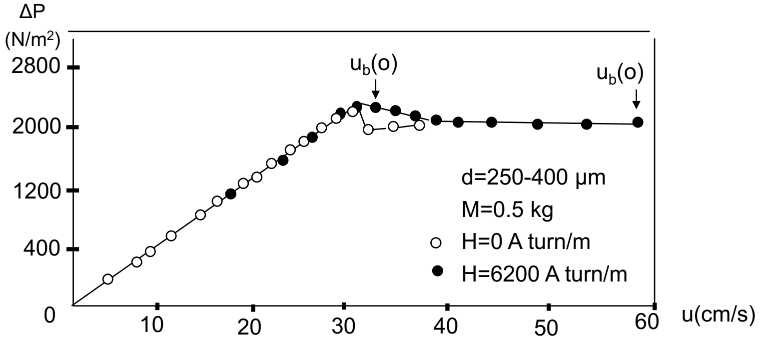


Fig. 5. Magnetically stabilized Fluidized bed behavior and transition velocity

A better knowledge of the structure of this type of fluidized bed (the stabilized bed) was achieved. The state of the bed could be described as falling between two limiting zones: the bed with particles situated at random with gas flowing though tortuous interstitial channels and the bed that forms ordered arrays of particles like chains with gas flowing straight through the rectilinear channels, (Fig. 6).

Applications were found in mixed systems containing magnetizable particles for the modeled, high-performance fluidized bed (Fig. 7). *A promising application was our incipient work on upgrading residual materials by thermal treatment in fluidized beds*. The mixtures consisted in refuse coal mixed with waste wood from different sources [14].

Sulfur abatement was efficiently achieved using a cheap catalyzer as an adsorbent, whose active component was iron oxide-based. The real problem that jeopardized the industrial application of this method was economy of scale. However, it gave us new insight into a complex system that is being incorporated into our current work to obtain clean hydrogen from waste materials. I consider this advance the result of the *evolution of several CAPE concepts and the hybridization of several techniques*.

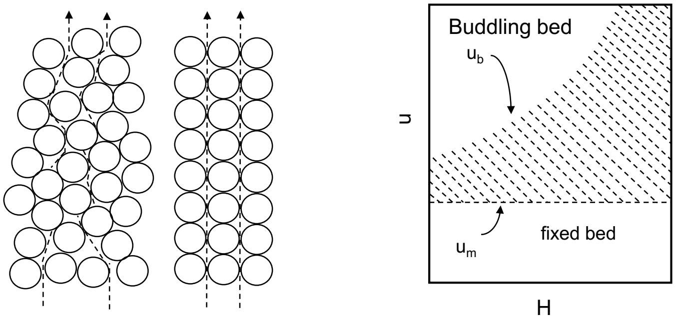


Fig. 6. Bed modeling: At left, spatial rearrangement of particles; at right, the three zone diagram

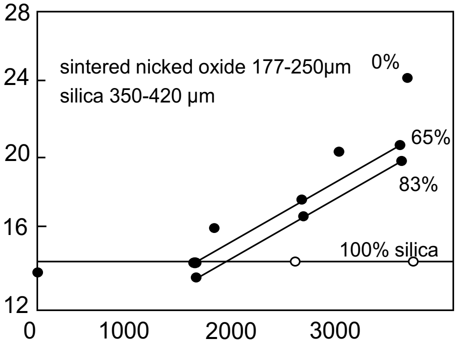


Fig. 7. Mixed particles systems applications

2.5 Modeling Batch processes

Back in the nineteen eighties, David Rippin whispered in my ear that "*the future is in batch*".

I will always be grateful to David for pointing me in the direction of a topic that at the time seemed an anachronism to engineers who were striving to achieve professional excellence by retrofitting batch designs into continuous operating processes. I was also very impressed by the amount of work already done by David, which he had written in German. He sent me his work in two big boxes, which I keep to this day. Most of this work had never been published, with the exception of that done on multi-batch and a few internal reports. This may also explain why we "started from the top", *as I was once told by Rex Reklaitis* at a meeting in Cambridge in 1988.

The truth of the matter is that after reading Rippin's material, I felt I had to start modeling the scheduling of a *multipurpose plant*. I was once again fortunate in that Manolo Lázaro was my first PhD student in the field of batch knowledge. He successfully identified the best production scheduling, out of the 451 feasible alternatives, for a real multi-purpose batch plant manufacturing three large volume products, being two of them dependent on production intermediates (Fig. 8) [15].

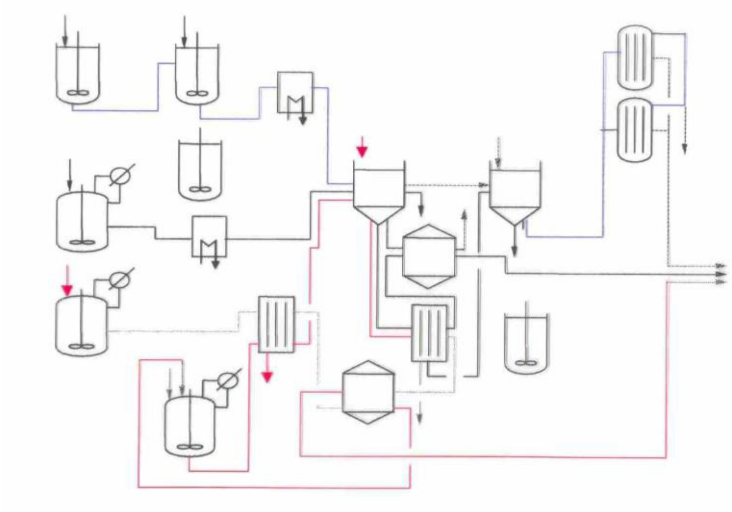


Fig. 8. Multipurpose batch plants planning and scheduling

David Rippin once called our work on batch modeling, and indeed, batch work in general, as "*filling in the holes*". This was at ESCAPE 2 in Toulouse, in 1992. He was essentially right, since rigorous batch models were almost non-existent and the complexity of the problem did not make it possible to find solutions for specific models in reasonable computing times.

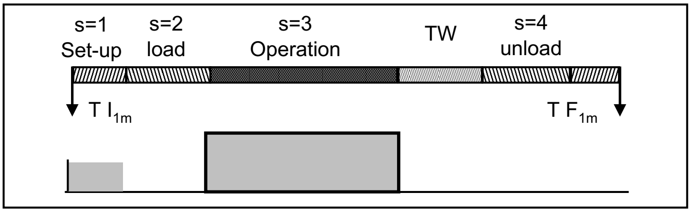


Fig. 9. Detailed scheduling model

For instance, it was not until 1993 that Moisès Graells [16] formulated an accurate representation of the subtasks examined in every batch process task (Fig.9). Obviously, the inclusion of this detailed representation of tasks in the mathematical production-scheduling model resulted in a highly complex formulation, and long computing times were necessary to solve it. Then a most complex **textile Company** manufacturing socks application came out. Specifically, the problem to solve includes planning for long- and short-term detailed scheduling for large parallel multiproduct facilities of a textile industry that manufactures 12,700 families of products, and whose main stage (called "Weaving") is constituted by 450 processing dedicated units working in parallel that require displacement and onsite installation for each family of products to achieve an optimal "chrono".

A Multi-objective set and the additional on-line information coming from actual plant operation allows any incident that occurs during the manufacturing to be adequately treated. Those two years (1992-93) *led to a breakthrough in the detailed modeling of a large-scale industrial application with satisfactory results* [17].

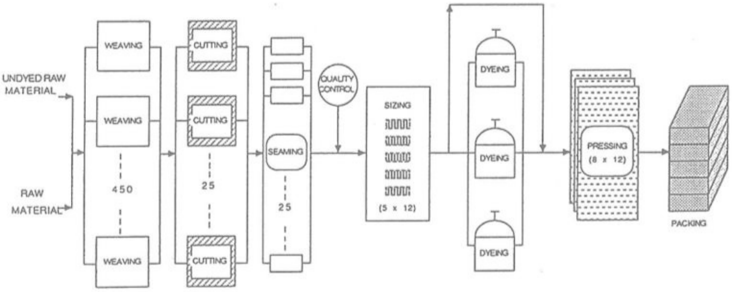
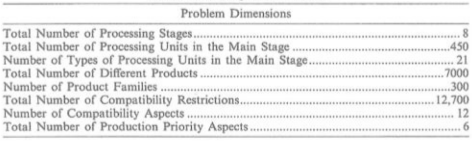


Figure 3. Production recipe for the test case.

Table 1. Flowshop characteristics



Problem Dimensions	
Total Number of Processing Stages	8
Total Number of Processing Units in the Main Stage	450
Number of Types of Processing Units in the Main Stage	21
Total Number of Different Products	7000
Number of Product Families	300
Total Number of Compatibility Restrictions	12,700
Number of Compatibility Aspects	12
Total Number of Production Priority Aspects	6

Fig. 10. Integrated planning and scheduling of a large industrial facility

Conclusions

I would like to end by saying that my instinct tells me that *breakthrough discoveries do not readily happen in engineering*, even more so in the case of Computer Aided Process Engineering (CAPE), as a second paper presented in CIMPS will corroborate. This is mainly *because new ideas* in this field *are continuously undergoing a process of dynamic development until they become sufficiently mature to be adopted by our industrial and social fabric, which is precisely the underlying essence of engineering*.

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