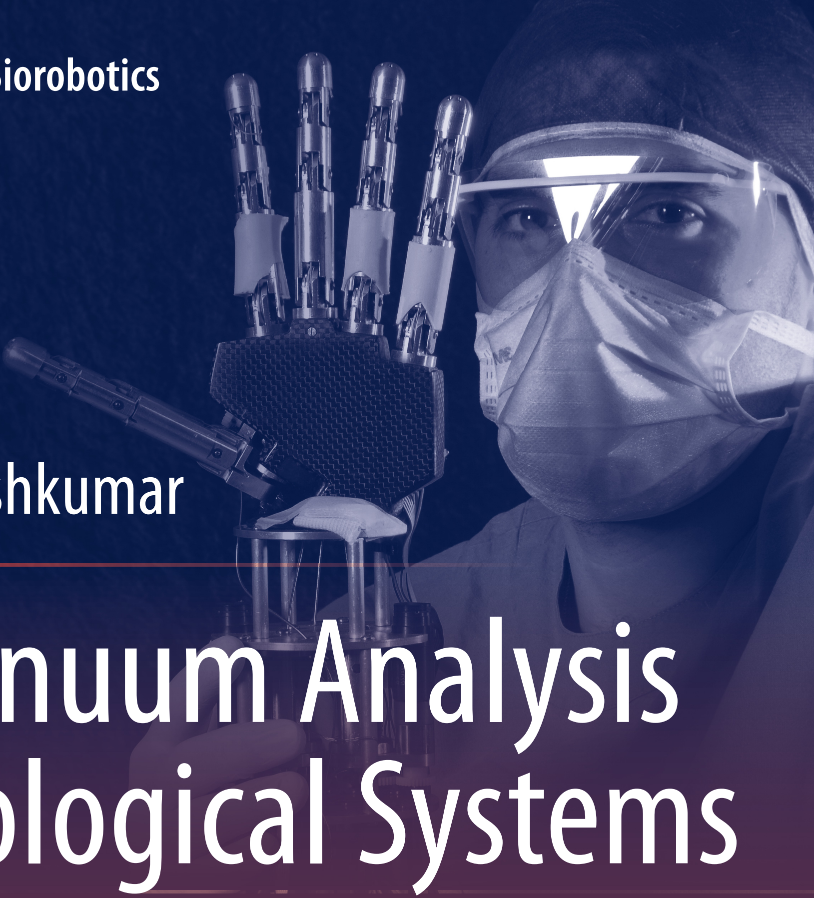
Biosystems & Biorobotics

G.K. Suraishkumar



Continuum Analysis of Biological Systems

Conserved Quantities, Fluxes and Forces

Springer

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Eugenio Guglielmelli, Campus Bio-Medico University of Rome, Rome, Italy
e-mail: e.guglielmelli@unicampus.it

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Aims & Scope

Biosystems & Biorobotics publishes the latest research developments in three main areas: 1) understanding biological systems from a bioengineering point of view, i.e. the study of biosystems by exploiting engineering methods and tools to unveil their functioning principles and unrivalled performance; 2) design and development of biologically inspired machines and systems to be used for different purposes and in a variety of application contexts. The series welcomes contributions on novel design approaches, methods and tools as well as case studies on specific bioinspired systems; 3) design and developments of nano-, micro-, macro- devices and systems for biomedical applications, i.e. technologies that can improve modern healthcare and welfare by enabling novel solutions for prevention, diagnosis, surgery, prosthetics, rehabilitation and independent living.

On one side, the series focuses on recent methods and technologies which allow multi-scale, multi-physics, high-resolution analysis and modeling of biological systems. A special emphasis on this side is given to the use of mechatronic and robotic systems as a tool for basic research in biology. On the other side, the series authoritatively reports on current theoretical and experimental challenges and developments related to the “biomechatronic” design of novel biorobotic machines. A special emphasis on this side is given to human-machine interaction and interfacing, and also to the ethical and social implications of this emerging research area, as key challenges for the acceptability and sustainability of biorobotics technology.

The main target of the series are engineers interested in biology and medicine, and specifically bioengineers and bioroboticists. Volume published in the series comprise monographs, edited volumes, lecture notes, as well as selected conference proceedings and PhD theses. The series also publishes books purposely devoted to support education in bioengineering, biomedical engineering, biomechatronics and biorobotics at graduate and post-graduate levels.

About the Cover

The cover of the book series Biosystems & Biorobotics features a robotic hand prosthesis. This looks like a natural hand and is ready to be implanted on a human amputee to help them recover their physical capabilities. This picture was chosen to represent a variety of concepts and disciplines: from the understanding of biological systems to biomechatronics, bioinspiration and biomimetics; and from the concept of human-robot and human-machine interaction to the use of robots and, more generally, of engineering techniques for biological research and in healthcare. The picture also points to the social impact of bioengineering research and to its potential for improving human health and the quality of life of all individuals, including those with special needs. The picture was taken during the LIFEHAND experimental trials run at Università Campus Bio-Medico of Rome (Italy) in 2008. The LIFEHAND project tested the ability of an amputee patient to control the Cyberhand, a robotic prosthesis developed at Scuola Superiore Sant’Anna in Pisa (Italy), using the tf-LIFE electrodes developed at the Fraunhofer Institute for Biomedical Engineering (IBMT, Germany), which were implanted in the patient’s arm. The implanted tf-LIFE electrodes were shown to enable bidirectional communication (from brain to hand and vice versa) between the brain and the Cyberhand. As a result, the patient was able to control complex movements of the prosthesis, while receiving sensory feedback in the form of direct neurostimulation. For more information please visit http://www.biorobotics.it or contact the Series Editor.

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CONSISTING OF KNOWLEDGE
ANAMAYA

G.K. Suraishkumar
Department of Biotechnology
Indian Institute of Technology Madras
Sophisticated Analytical Instr. Facility
Chennai
India

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Foreword

This textbook should be a welcome addition for teachers and students of biotechnology. On the first few pages one encounters words like metabolic pathways, enzymes, genes, and aerobic bioreactors. This should suggest to typical readers that this book will be “bio-friendly”.

The general outline of the book is sensible, with mass transport, momentum transport, energy transport, and charge transport being discussed in that order. The book concludes with a chapter on combined methods of transport. Some topics have been omitted from the book, and wisely so. There is only a limited discussion of radiative heat transfer, a very complex subject that is perhaps of marginal interest in biology and physiology. There is no discussion of the kinetic theory of the transport properties, and this topic would be only of marginal interest to the intended readership.

There are problems at the end of each chapter dealing with biological problems, as well as in the text itself. At the end of Chapter 4, there is even a “Harry Potter” problem to provide a bit of diversion. There are also some open-ended problems at the ends of chapters, which should provide material for group or individual projects.

The author has provided units for all quantities introduced, and this should be particularly appreciated by the students. The notation is standard throughout, so that the reader will have no difficulty in consulting other textbooks and handbooks as the need may arise.

A rather complete appendix on vector and tensor operations appears at the end of the book. Here, and throughout the text, standard Gibbs notation is used. This will be particularly helpful for any student who has forgotten the definitions of the various “del” operations.

It is a pleasure to recommend this well-balanced and practical volume.

Prof. R.B. Bird
University of Wisconsin-Madison
1415 Engineering Drive, Madison, WI 53706, USA

Preface

It was a bright morning in December 2007, when one of my colleagues walked in to my sun-lit office and threw a tantrum that he would not teach a course that he had earlier agreed to teach in the Republic (January-May) 2008 semester. Unlike in many parts of the world, the seasons in our part of the country can be only described as hot, hotter, and hottest. Therefore, I use two major political events of the country to distinguish between the two semesters, at least in my course material – the 'Republic semester', that contains the Republic day (26th January) and the 'Independence semester' containing the Independence day (15th August).

Back to the sun-lit morning in 2007: the reasons given by the colleague for not wanting to teach the course were, at best irrational. I had to deal with it because I was the Department Head then. I feel fortunate and privileged to have been given two opportunities to significantly contribute to the set-up of academic departments – as the first formal head of the Department of Biotechnology at the Indian Institute of Technology (IIT) Madras (2005–2008), and again as the first head of the Department of Biotechnology and Biomedical Engineering at the new IIT at Hyderabad (2009–2011). Setting-up a department so that its foundations are strong and deep which would enable its significant contributions to an evolving field in the future was indeed an exciting task. The related thoughts and converting those to actions, with the support of most faculty members in the department, were exhilarating, despite minor irritants such as dealing with a few irrational, politicaster colleagues.

I realised that it would be best not to insist that the colleague teach that course, to spare the students who would be taking the course. So, I started to look for others in the department who could teach the course, but found none, as the teaching duties were agreed upon 9 months prior to that time, and they were all set to teach their assigned courses. The course for which I was trying to find a lecturer was unit operations and transport processes, which was taught from a unit operations perspective by the colleague who threw the tantrum. Being in a mind-set of getting into new things because of the involvement with setting up a new department, I thought to myself, 'how bad can teaching transport be?', although I had never taught transport earlier, and my research had an experimental base. Also, I was in my final year as the department head, with a clear realisation that I had done my best in whatever I could do for setting up good initial conditions for the department, and now, the department had to come up on its own. With that, I jumped into the deep end of the pool and decided to teach that course myself in the next semester that was beginning in a few days, and it is from the distils from this course that this book originated.

I did not want to teach transport from a unit operations perspective as the earlier person had done because that would seriously limit the confidence of the students when they analyse new situations, especially in an evolving field such as biological engineering. I had invested significant time in thinking about and working on a curriculum for biological engineering that was emerging at that time. I had realised that a good engineering curriculum emphasises imparting the necessary knowledge in a way that the students understand the knowledge, and use it toward analysis and design of appropriate systems. Thus, for example, in a biotechnology/biological engineering/related bio…-engineering curriculum there need to be courses that either separately or together cover knowledge, understanding, analysis and design of the biological systems.

Therefore, during the first offering of the course in the Republic 2008 semester, I taught the course the way I learnt transport over many years, starting with an initial exposure through a course, and later, through osmosis and occasional use in research. The paradigm-shifting, classic book by Bird, Stewart and Lightfoot was the base text, and I made up the examples with a biological flavour from my experiences and research. I also found the book, *Transport Phenomena in Medicine and Biology* by M.M. Lih, to be useful. As I taught the course that semester, I realised that momentum transport was a little too abstract for first mention to students. The mass transport aspects are usually easy to intuitively grasp, and hence it seemed a good candidate with which the transport discussion could be begun. Further, the concept of charge conservation/transport, which is an important principle for biological systems because many biological entities are charged, is not explicitly covered in any other book of this kind, especially in the context of forces and fluxes. In addition, I realised through experience that it is better to introduce the fluxes resulting from primary driving forces, before the fluxes that result under the simultaneous action of more than one driving force. This approach, and the consequent ‘flow’ of material, provided a better understanding of the relevant principles to the students.

I also realised that about 80% of the students in a typical undergraduate class in biotechnology are not naturally talented in mathematics (e.g. they are unable to foresee the results of multiple sequential steps), and spend a lot of time in trying to understand how the various mathematical steps in a textbook are arrived at; the typical textbook usually does not elaborate the intervening steps in a derivation. A significant percentage of interested students in a typical class get frustrated when they are unable to work out the mathematics. Thus, if the mathematical steps are explicitly shown, the appreciation for the rigour in the subject becomes better to an average student. Also, it would assure such students that it is possible to master the mathematics aspect through effort and focus. Of course, it may be boring to a student who is naturally talented in mathematics (less than 20% in a typical undergraduate class), and such students can be requested to skip the detailed steps.

The above were incorporated the next time the course was taught, and significantly improved upon the third time. It struck me during the Republic 2009 semester that the above could be disseminated to a larger audience, and the first manuscript was ready in the Republic 2010 semester. I felt that it was good to get the students’ perspective on the exercise problems, and assigned the same as a group exercise to students in consecutive years, with a 10% weightage toward the final grade. The names of the students who suggested/formulated the exercise problems that were selected for inclusion in this book are given just after the exercise problems in each chapter.

I have an interest in the learning process and do experiments on the same. Some worthwhile experiments have been better disseminated, and one such is the CFA exercise. CFA stands for choose, focus, analyse, respectively, which is a completely open-ended exercise designed to develop some desirable skills in students. Students needed to choose a problem of relevance to industry or any human endeavour and analyse it using the principles learned in class. The evaluation was based on originality in approach, 15%, focus level, 15%, depth of analysis, 20%, quantum of work, 20%, original contribution, 20%, and presentation (mainly communication) 10%. A concise report in the format that the student thought would best communicate the work was needed to be submitted a week before the last day of classes. The students were told that it will help if the problem is chosen well in advance (within the first four weeks) and sufficient time, distributed throughout the course duration, is devoted. My students fondly remember this exercise even after 15 years of having done them because they learnt best through that exercise. Some of those exercises have been included in most chapters in the book.

This book aims to fill the need for a comprehensive book on the analysis of biological systems in the continuum regime, in the context of forces and fluxes, to provide the student with the required skills to think-out-of-the-box in novelty requiring situations at one end, to a full appreciation of the relevant principles and its interconnections, at the other end. Also, it aims to be useful to industry personnel as a reference for the relevant principles. In the academia, the book can be used as a text for a variety of related courses in a biological engineering/biotechnology curriculum, such as momentum, heat and mass transfer, transport processes, and others. The material can be taught comfortably in a one semester 4 credit course in the fourth or the fifth semester. The instructors, after covering the basic concepts in the chapters, two to five, can choose the relevant combinations of forces and fluxes from the examples given in the sixth chapter. The material in the first half of the first chapter is usually covered in great detail in an earlier course, say material and energy balances. The instructors can use that material to review the earlier course, and introduce the material balance formulations for specific use in this course, may be in about three 50-minutes classes.

I would like to acknowledge the following people for their input and support toward this book:

- All my students who took the course over the past six years, and have thus provided valuable input
- Archanaa S. and Sandhya Moise, who first converted my hand-written notes to a soft copy, Srivatsan, who drew some charts, and Sukanya Moudgalya, who provided useful feedback

- Professor Robert Byron Bird who wrote the foreword – I am truly amazed at the ability and commitment of this legend at his age; he read the entire 350+ pdf pages of the manuscript in three days flat, and gave excellent input to improve the book, including pointing out errors where C_V was used in the place of C_P!
- Lokeshwarri, my wife, who in her typical quiet way, whole-heartedly supported this effort. At one time, she was more interested than me in seeing the book published, and actively sought information on suitable publishers from her friends
- Sreshtaa, my daughter, who provided me an opportunity to think from a different perspective that was essential for the book to turn out the way it has
- My professional friends at IIT Bombay who supported me in this long journey to publish
- My colleagues at the Sophisticated Analytical Instrument Facility, Chennai at IIT Madras, for which I was responsible; it was during that period (2009–2013) when much of the actual writing took place. They cooperated well with my timings – I wrote in the mornings closeted in my office, and was available for the needed meetings only in the afternoons
- My primary school classmates from the Christ King Primary School, Tambaram, Chennai – getting back in touch with them, some friends much more than the others, through the facebook group that I initiated, and email messages, put me in touch with my childhood self, and that was of crucial importance for me. It is amazing how some special bonds last more than 36 years even without being in touch!

In addition, thanks for their efforts are due to Anamaya Publishers, Mr. Manoj Karthikeyan, and the entire publication team including the technical editor, Ms. Jebah, who seemed to be involved with this book, and has done an excellent piece of work.

G.K. Suraishkumar

Contents

Part I
Mass Conservation

Chapter 1
The Principle

There are some physical quantities that are conserved in nature. Examples include mass (conserved in many cases of engineering interest), energy, momentum, angular momentum, charge and spin. Conserved quantities are a boon when appropriate systems need to be designed and analysed. This is because generally, in most cases, when dealing with equations of the above quantities, the left-hand side equals the right-hand side (LHS = RHS), i.e. the above quantities remain unchanged, for example, in a process.

In this book, we will look at the consequences when conservation of the above mentioned physical quantities are invoked in the context of 'forces', and the relevant 'fluxes' that result from the forces in biological systems. The meaning of the terms 'forces' and 'fluxes' will become clearer as we go along.

Let us begin with the principle of conservation of mass and move, as needed, to conservation of momentum, energy, and charge.

1.1 Conservation of Mass

We know from the physics we learnt at high school that 'mass can neither be created nor destroyed'. With more in-depth knowledge, especially about mass to energy conversion in nuclear reactions, we understood the limitation of the above conservation principle, and modified the principle to state that 'mass can neither be created nor destroyed when we consider non-nuclear processes'. In this book, we limit ourselves to non-nuclear processes (there is mass to energy conversion in nuclear processes) that occur at velocities much less than the velocity of light to neglect mass dilation effects, and hence we can be comfortable using the simpler mass conservation principle.

How do we use the mass conservation principle?

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1.1.1 A Convenient Form of the Equation of Mass Conservation

Let us first generate the relevant equation of mass conservation for a system, which is easier to use. Why are we doing it for a *system*? If we do it for a system, the equation becomes general enough to use under a large variety of situations, as long as the *system* is appropriately defined. It may be recalled from a fundamental course in thermodynamics that a 'system' is an aspect on which we choose to focus our attention. It could be a biological cell, or a tiny part of a cell, at one end of the range, to a vessel in a process plant or the entire process plant itself, at the other end of the range of length scales with which we are concerned in this book.

The system can be as large as one's imagination permits, according to the needs of the analysis, but it cannot be smaller than the space that would allow us to consider the material as a continuum, if we need to apply the principles of analysis given in this book. 'Continuum' refers to the situation when there are a large number of unitary particles (say molecules) per unit volume, and the substance under consideration can be considered as a continuous one. When the number of molecules per unit volume decreases below a certain value, the properties of the substance, say density, *at the same position*, will fluctuate widely with time. Then, the substance cannot be considered as being continuous, and we are in the non-continuum regime. It needs to be understood that the properties of a substance can vary across the substance, i.e. be a function of the position; such a substance is merely heterogenous in nature—this does not preclude the application of the continuum principle for the analysis of such a substance. Further, in biological systems, as a rule of thumb, if the number of molecules under consideration, say inside the cell, is less than about 100, we cannot use the continuum analysis principles. For example, when we are studying the interactions between proteins or between DNA and proteins, the continuum approach will not be suitable. Nevertheless, methods of statistical mechanics can be employed in such cases. This book will limit itself to the continuum regime.

Let us indicate the boundaries of our system by a dashed line, as shown in Fig. 1.1.1-1.

Let there be n input streams, m output streams and k components. There are only five things that can happen to any component of interest in the context of a system:

1. It can enter (cross the system boundaries into) the system or be an 'input' to the system (I)
2. It can exit (cross the system boundaries out of) the system or be an 'output' from the system (O)
3. It can be generated as a result of say, a reaction in the system (G)

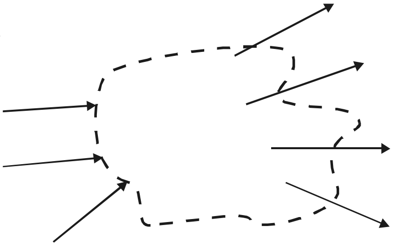


Fig. 1.1.1-1 Representation of a system with inputs and outputs

4. It can be consumed as a result of say, a reaction in the system (*C*)
5. It can accumulate in the system (*A*)

The quantities shown in brackets above, *I*, *O*, *G*, *C* and *A*, denote the amounts of the species undergoing various fates in the context of the system.

Intuitively, we can write the following algebraic relationship between the fates:

$$I + G - O - C = A \tag{1.1.1-1}$$

As may already be known, the time rates or amounts per time are more important to engineers than the actual amounts. For example, let us say that we are interested in determining the water level in a 50 l bucket with water at a certain time after we start filling it from a tap. Let us make it slightly complex by adding that the bucket was initially half full, and that it has a hole at the bottom through which water flows out. In such cases, the amounts or volumes are not of interest. It is the flow rates of input (tap) and output (hole) that are of interest.

If we represent the time rates of *I*, *G*, *O* and *C* with a dot above the respective symbols, and the time rate of *A* by a derivative, a differentiation of Eq. 1.1.1-1 with respect to time yields

$$\dot{I} + \dot{G} - \dot{O} - \dot{C} = \frac{\partial A}{\partial t} \text{ or } = \frac{dA}{dt} \tag{1.1.1-2}$$

We represent the accumulation rate of *A* explicitly by a derivative only for ease of direct application of the equation for analysis. In the above equation, we converted the partial derivative into a total derivative, because we consider the system to be a well-mixed one (no variation with position). Also note that the quantities on the LHS may be constant or may vary with time, when a large time scale is considered for integration.

1.2 Application of Mass Conservation to a Biological Cell: Metabolic Flux Analysis

We know from a basic course in biochemistry that there exist thousands of bioreaction pathways in the cell, and that they are crucially responsible for the functioning of the cell. Manipulation of metabolic pathways to improve bio-product yields is an age-old concept. For example, many empirical techniques such as random mutagenesis, medium formulations, and *r*-DNA technology that is based on a better understanding than the earlier mentioned techniques, are all directed toward manipulation of metabolic pathways. Nevertheless, the choice of the gene to be manipulated to improve or suppress the needed enzymes, or the choice of the substrate to be provided was decided through extensive experiments or by an intuitive feel. Nowadays, metabolic flux analysis (MFA) provides us with a more accurate tool to make a reasonably rational choice of enzymes/genes to manipulate or appropriate substrate to provide. It is based on the principle of mass conservation applied on the cell, by considering the cell as the system of interest. Here, our interest is to represent the rates of the various relevant reactions inside the cell in a useful form/framework. Further analysis is required to make sense of, or to use the representation. Such details are beyond the scope of this text. However, they can be found in books on metabolic analysis such as that by Stephanoupoulos et al. (1998).

To illustrate the basis for the method, let us consider a few reactions that occur in the cell, and represent them as shown in Fig. 1.2-1. Let us consider the cell as our system, and let us indicate the system boundaries (assume it to be the surface of the cell) by dotted lines as shown in Fig. 1.2-1. From the figure, it can be seen that S_o, C and D are extracellular metabolites; S, A and B are intracellular metabolites. Let the rates of the individual steps, r_0, r_1, r_2, r_3 and r_4 be represented as mmole per second, or in more practical terms, mmole (g cell)$^{-1}$ s^{-1}. For historical reasons, the above rates are referred to as metabolic 'fluxes', although the term, 'flux', refers to a different quantity in an engineering context, as we will see in Chapter 2.

Let us first consider the metabolite A. A material balance on the metabolite A, using the Eq. 1.1.1-2 gives

$$\dot{I}_A + \dot{G}_A - \dot{O}_A - \dot{C}_A = \frac{dA_A}{dt} \tag{1.2-1}$$

which can be written by combining the terms differently, as

$$(\dot{G}_A - \dot{C}_A) - (\dot{O}_A - \dot{I}_A) = \frac{dA_A}{dt}$$

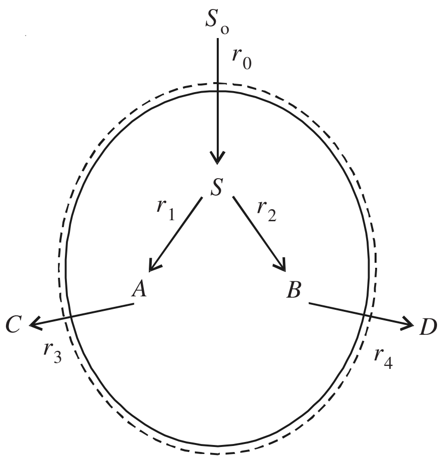


Fig. 1.2-1 An example of a framework for metabolic flux analysis

or as

$$(\text{Net generation rate})_A - (\text{Net transport rate})_A = \frac{dA_A}{dt} \tag{1.2-2}$$

A similar balance can be written for each of the metabolites. Thus, the number of balances equals the number of metabolites.

Let us write material balances on intracellular variables S, A and B, by considering the cell as the system. Let us consider r_0 as the generation rate. It can be considered as the transport rate across the cell envelope too. However, we need to account for it only once, i.e. either as a generation rate or as a transport (input) rate, not both. In terms of the rates r_0 to r_4, we can write the balances using Eq. 1.2-1 as:

$$r_0 - r_1 - r_2 = \frac{dS}{dt} \tag{1.2-3}$$

$$r_1 - r_3 = \frac{dA}{dt} \tag{1.2-4}$$

$$r_2 - r_4 = \frac{dB}{dt} \tag{1.2-5}$$

Let us write material balances on extracellular variables, S_o, C and D, by considering cell surroundings as our system of interest. Different systems can be considered for different balances, as long as one is careful not to mix up the systems while writing each balance (this happens to be a common error, and needs to be considered while checking the balances).

$$-r_0 = \frac{dS_o}{dt} \tag{1.2-6}$$

$$r_3 = \frac{dC}{dt} \tag{1.2-7}$$

$$r_4 = \frac{dD}{dt} \tag{1.2-8}$$

The above equations can be written in a compact form using matrices as:

$$\begin{bmatrix} -1 & 0 & 0 & 0 & 0 \\ 1 & -1 & -1 & 0 & 0 \\ 0 & 1 & 0 & -1 & 0 \\ 0 & 0 & 1 & 0 & -1 \\ 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 1 \end{bmatrix} \begin{bmatrix} r_0 \\ r_1 \\ r_2 \\ r_3 \\ r_4 \end{bmatrix} = \frac{d}{dt} \begin{bmatrix} S_o \\ S \\ A \\ B \\ C \\ D \end{bmatrix} \tag{1.2-9}$$

or

$$\tilde{S} \,.\, \tilde{r} = \frac{d}{dt} \tilde{x} \tag{1.2-10}$$

where $\tilde{S}$ is stoichiometric matrix, $\tilde{r}$ is reaction rate vector and $\tilde{x}$ is state vector (vector of state variables).

Equation 1.2-10 that can be used to quantify metabolic fluxes (note as mentioned before that the term ‘flux’ in the metabolic context, is historically used to denote rates. Its units are moles time^{-1} or mass time^{-1}. In the next chapter, we will look at a more consistent definition of flux) based on experimental data, with further assumptions such as pseudo-steady state, can also be utilised for various kinds of analysis such as nodal rigidity analysis, identification of alternate pathways in the cell, calculation of maximum theoretical yields, genome-scale analysis, and others. The reader is referred to specialised texts on metabolic analysis (e.g. Stephanoupoulos et al. 1998) for details.

1.3 Application of Mass Conservation to Macroscopic Systems

Now, let us look at how the mass conservation principle can be applied to get useful information at a larger length scale, around a biologically relevant macro-system. Consider a bioreactor, which, as may be known, is a controlled and instrumented vessel that is used for making bio-products. Let us focus on one aspect of an aerobic bioreactor, i.e. oxygen supply. An aerobic bioreactor, as can be recalled, is one that employs oxygen requiring (aerobic)

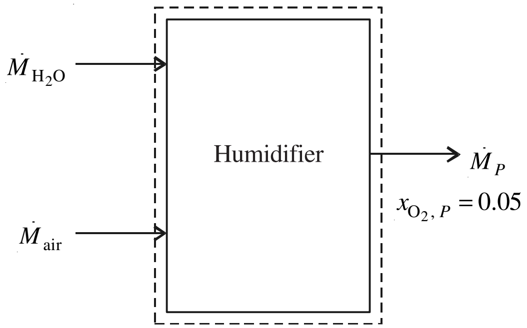


Fig. 1.3-1 The system considered for analysis

microorganisms or higher cells to make bio-products. Air is usually the source of oxygen, and it needs to be humidified before entry into the bioreactor to minimise evaporation loss of water from the bioreactor contents. A humidifier is used to achieve the same.

The humidifier is fed with dry air (with no water vapour; it is removed during the processing of air to avoid contamination of the bioreactor) and clean liquid water. The liquid water flow rate is 18 cc min^{-1}. If 5 mole % of oxygen is needed in the output stream of the humidifier for supply to the bioreactor, let us determine that molar rate at which air should be supplied to the humidifier, when it operates at steady state.

First, let us represent the situation using a figure, along the values of interest from the problem statement (Fig. 1.3-1). The molar flow rates of streams are represented by $\dot{M}$ and the mole fraction in a stream is represented by x.

Let us consider the humidifier as our system, and let us work with moles. We prefer to work with moles because of the requirements of the problem. Mole = mass/molecular mass, and if there is no change in the species, say due to a reaction during the process, the mole balances on individual species are as good as the mass balances. Nevertheless, note that mass is more general, and when unsure, it is safe to balance masses.

We also know that dry air is made of 21 % oxygen and 79 % nitrogen by volume or mole; let us ignore the other minor components of air for this problem. Thus, the molar flow rates of oxygen and nitrogen in the air stream can be written as

$$\dot{M}_{O_2,\,\mathrm{air}} = 0.21\,\dot{M}_{\mathrm{air}} \tag{1.3-1}$$

$$\dot{M}_{N_2,\,\mathrm{air}} = 0.79\,\dot{M}_{\mathrm{air}} \tag{1.3-2}$$

The flow rate of H_2O is 18 cc min^{-1} = 18 g min^{-1} (since the density of water can be taken as 1 g cc^{-1}) = 1 mole min^{-1} (molecular mass of H_2O = 18).

Now, let us perform the mass balances to find the molar flow rate of air. Note that since we are doing the analysis at steady state, all the time derivatives will be zero.

$$\dot{I}+\dot{G}-\dot{O}-\dot{C}=\cancelto{=0(SS)}{\frac{dA}{dt}}$$

O_2 Balance

$$\dot{M}_{\mathrm{O_2,\,in}}+\cancelto{=0}{\dot{M}_{\mathrm{O_2,\,generated}}}-\dot{M}_{\mathrm{O_2,\,out}}-\cancelto{=0}{\dot{M}_{\mathrm{O_2,\,consumed}}}=0 \qquad (1.3\text{-}3)$$

$$0.21\,\dot{M}_{\mathrm{air}}-0.05\,\dot{M}_P=0$$

or

$$\dot{M}_P=\frac{0.21}{0.05}\dot{M}_{\mathrm{air}}$$

Total Mole Balance

Since there is no generation or consumption of moles in this process, Eq. 1.3-3 is valid. Thus

$$(\dot{M}_{\mathrm{air}}+\dot{M}_{\mathrm{H_2O}})-\dot{M}_P=0 \qquad (1.3\text{-}4)$$

$$\dot{M}_{\mathrm{air}}+1-\frac{0.21}{0.05}\dot{M}_{\mathrm{air}}=0$$

$$\dot{M}_{\mathrm{air}}=0.31\ \mathrm{mol\ min^{-1}}$$

From experience, it is known that significant practice is needed by average students before they feel comfortable applying the material balance principle even to macroscopic systems, although the principle and the mathematics involved are simple. The above sections are intended to serve as examples of the material balance principle being applied to biological systems. Some more exercises for practice are given toward the end of this chapter.

1.3.1 Challenges in Oxygen Supply to Bioreactors

Industrial bioreactors are large vessels, typically 10,000 to 100,000 litres. Cells multiply in these vessels to reach high concentrations – ten billion (10^{10}) cells per ml is typical for microorganisms such as bacteria, which measure about 2 microns in size – and as a result of a complex set of reactions occurring inside them, make the product of interest. For many cells, oxygen is a requirement for these reactions to occur.

Nevertheless, supplying oxygen at adequate levels to the bioreactor has remained a challenge. This is because the normal mode of oxygen supply by bubbling air (aeration), is inadequate to meet the oxygen needs of the cells. Augmentation with pure oxygen is usually expensive. Further, the normal aeration and agitation levels in the bioreactor can result in high shear (forces which can tear cells apart) levels. Therefore, a related challenge is that of providing a gentle enough environment in the bioreactor with minimum shear for the cells to multiply and make products optimally.

The liquid phase oxygen-supply strategy (LPOS) can effectively overcome both the above challenges (Sriram et al. 1998). It is also relatively inexpensive. The LPOS involves providing oxygen by using a ‘green chemical’, hydrogen peroxide, which is added according to the need. The added hydrogen peroxide is converted to oxygen using an enzyme, catalase, which is made by the cells, themselves. Although hydrogen peroxide is toxic at high concentrations, the low concentrations employed in the LPOS do not harm the cells at all. While studying and analysing the LPOS (Sriram et al. 1998), material balances play an important role, as may be evident from some of the exercises at the back of the book.

1.4 Useful Forms of Mass Conservation in Fluid Systems

1.4.1 What is a Fluid?

A fluid – either a gas or a liquid – is a substance that takes the shape of the vessel containing it. All real fluids have a property called viscosity associated with them which determines their behaviour under many circumstances. We will look at this aspect in more detail in a later chapter.

1.4.2 Useful Derivatives

Before we look at mass conservation in fluids, let us familiarise ourselves with the kinds of derivatives that we need. Let us say that we are interested in studying the effect of currents on fish concentration in the ocean. We are equipped with a sonar based fish counting device on a motor boat with strong anchors.

The fish concentration c, is a function of space (x, y, z) and time (t). If we drop our strong anchors, and count the fish, we observe the concentration at a fixed position. The variation in fish concentration with time is given by

$$\left(\frac{\partial c}{\partial t}\right)_{x,y,z} \tag{1.4.2-1}$$

i.e. partial derivative of c with respect to t, at constant x, y, z.

Typically, x, y, z are not explicitly shown as constants in the partial derivative, unless required to avoid confusion.

Now, if we raise the anchor, start the engine of the motor boat and move about in the ocean, the time rate of change of c is given by the application of the chain rule as

$$\frac{dc}{dt}=\frac{\partial c}{\partial t}+\frac{\partial c}{\partial x}\frac{\partial x}{\partial t}+\frac{\partial c}{\partial y}\frac{\partial y}{\partial t}+\frac{\partial c}{\partial z}\frac{\partial z}{\partial t}$$

Since, $c = f(t, x, y, z)$, but $x = f(t)$, $y = f(t)$, $z = f(t)$, i.e. only functions of t, we can replace the partial derivatives with t by total derivatives.

$$\frac{dc}{dt}=\frac{\partial c}{\partial t}+\frac{\partial c}{\partial x}\frac{dx}{dt}+\frac{\partial c}{\partial y}\frac{dy}{dt}+\frac{\partial c}{\partial z}\frac{dz}{dt} \tag{1.4.2-2}$$

Here, $\frac{dx}{dt}, \frac{dy}{dt}$ and $\frac{dz}{dt}$ are components of the boat velocity and, $\frac{\partial c}{\partial x}, \frac{\partial c}{\partial y}$ and $\frac{\partial c}{\partial z}$ are components of the concentration changes with respect to the boat's position at a certain time. Thus, the total derivative reflects the concentration changes with respect to both time and the observer's position.

Now, suppose we shut off the engines, but do not drop anchor. Then, we move about with the velocity of the stream/current/region, $\vec{v}$ (local velocity). When this happens, the change in fish concentration with time will depend on the local velocity, $\vec{v}$. Such a derivative is called 'time derivative for the motion' or 'substantial derivative'. It is expressed as

$$\frac{Dc}{Dt} = \frac{\partial c}{\partial t} + v_x \frac{\partial c}{\partial x} + v_y \frac{\partial c}{\partial y} + v_z \frac{\partial c}{\partial z} \qquad (1.4.2\text{-}3)$$

where v_x, v_y, v_z are the components of the local velocity $\vec{v}$.

This can be expressed more compactly in vector notation as

$$\frac{Dc}{Dt} = \frac{\partial c}{\partial t} + (\vec{v}\,.\vec{\nabla} c) \qquad (1.4.2\text{-}4)$$

To understand the second term on the RHS in Eq. 1.4.2-4, note that

$$\vec{v} = \vec{\imath} v_1 + \vec{\jmath} v_2 + \vec{k} v_3$$

and

$$\nabla = \vec{\imath}\frac{\partial}{\partial x} + \vec{\jmath}\frac{\partial}{\partial y} + \vec{k}\frac{\partial}{\partial z}$$

$\vec{\imath}, \vec{\jmath}$ and $\vec{k}$ are the unit vectors in the x, y and z directions, respectively.

Thus, a dot product of the above vectors, which is done by a term-by-term multiplication of the coefficients for the coefficients of the resultant vector, would yield the second term on the RHS of the Eq. 1.4.2-3.

When we take the 'time derivative following the motion', we follow an approach called the 'Lagrangian approach' (after the French mathematician, J.L. Lagrange) where we study a tiny element of fluid that follows the motion of the main body of the fluid. The shape and volume of the element and the density of the material contained in the element can be different at different points of the flow, but the mass within the element remains constant.

When the system is a small element that is *fixed* in space, and is of constant volume, the approach is called Eulerian (pronounced Oyler, after the Swiss mathematician and physicist, Leonard Euler). We will predominantly use the Eulerian approach in this text.

1.4.3 Equation of Continuity for a Single Component System

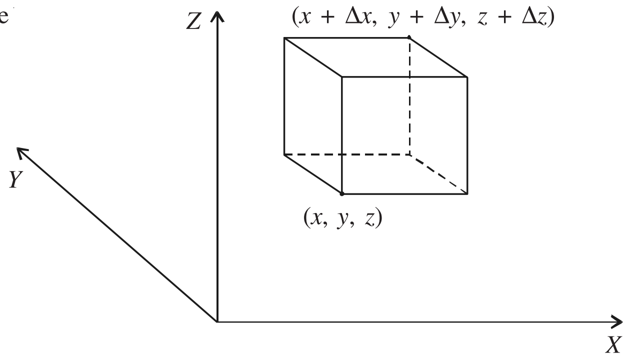
Let us consider a fixed volume element in the space of volume $\Delta V = \Delta x\, \Delta y\, \Delta z$ through which the fluid flows. Consider a right-handed coordinate system for our analysis as shown in Fig. 1.4.3-1.

Let us use the general material balance equation that we have developed earlier in this chapter.

$$\frac{dA}{dt} = \dot{I} + \dot{G} - \dot{O} - \dot{C} = \dot{I} - \dot{O} + (\dot{G} - \dot{C}) = \dot{I} - \dot{O} + \dot{P} \qquad (1.4.3\text{-}1)$$

where $\dot{P}$ is the net rate of production.

Fig. 1.4.3-1 A volume element in a right-handed coordinate system



Since we are considering total mass here (no generation and consumption), the equation reduces to

$$\frac{dA}{dt} = \dot{I} - \dot{O} \tag{1.4.3-2}$$

This is a three-dimensional flow. Therefore, we need to consider the contributions from all directions. Let us do them one by one.

Before that, let us note that ρ (kg m^{-3}) × v (m s^{-1}) = mass flux ρv (kg m^{-2} s^{-1}). Thus

$$\text{Rate of mass in through the face at } x = (\rho v_x)|_x \, \Delta y \Delta z$$

$$\text{Rate of mass out through the face at } x + \Delta x = (\rho v_x)|_{x+\Delta x} \, \Delta y \Delta z$$

$$\text{Rate of mass in through the face at } y = (\rho v_y)|_y \, \Delta x \Delta z$$

$$\text{Rate of mass out through the face at } y + \Delta y = (\rho v_y)|_{y+\Delta y} \, \Delta x \Delta z$$

$$\text{Rate of mass in through the face at } z = (\rho v_z)|_z \, \Delta x \Delta y$$

$$\text{Rate of mass in through the face at } z + \Delta z = (\rho v_z)|_{z+\Delta z} \, \Delta x \Delta y$$

$$\begin{aligned}\text{Rate of mass accumulation within the volume element} &= \frac{\partial(\rho V)}{\partial t}\\ &= \frac{\partial \rho(\Delta x \Delta y \Delta z)}{\partial t}\\ &= \Delta x \Delta y \Delta z \frac{\partial \rho}{\partial t}\end{aligned}$$

Therefore, the mass balance using Eq. 1.4.3-2 yields

$$\begin{aligned}\Delta x \Delta y \Delta z \frac{\partial \rho}{\partial t} = \Delta y \Delta z &\left\{(\rho v_x)|_x - (\rho v_x)|_{x+\Delta x}\right\}\\ &+ \Delta x \Delta z\left\{(\rho v_y)|_y - (\rho v_y)|_{y+\Delta y}\right\}\\ &+ \Delta x \Delta y\left\{(\rho v_z)|_z - (\rho v_z)|_{z+\Delta z}\right\}\end{aligned} \tag{1.4.3-3}$$

If we divide throughout by $\Delta x \Delta y \Delta z$, we get

$$\frac{\partial \rho}{\partial t}=\frac{1}{\Delta x}\left\{(\rho v_x)|_x-(\rho v_x)|_{x+\Delta x}\right\}+\frac{1}{\Delta y}\left\{(\rho v_y)|_y-(\rho v_y)|_{y+\Delta y}\right\}+\frac{1}{\Delta z}\left\{(\rho v_z)|_z-(\rho v_z)|_{z+\Delta z}\right\}$$

When we impose the limit of an infinitesimal volume, i.e. $\Delta x \to 0$, $\Delta y \to 0$ and $\Delta z \to 0$, we get

$$\frac{\partial \rho}{\partial t}=-\left(\frac{\partial}{\partial x}\rho v_x+\frac{\partial}{\partial y}\rho v_y+\frac{\partial}{\partial z}\rho v_z\right) \qquad (1.4.3\text{-}4)$$

In vector notation

$$\frac{\partial \rho}{\partial t}=-(\vec{\nabla}\,.\,\rho\vec{v}) \qquad (1.4.3\text{-}5)$$

Now let us go back to Eq. 1.4.3-4 and expand the RHS using chain rule

$$\frac{\partial \rho}{\partial t}=-\left[\rho\frac{\partial v_x}{\partial x}+v_x\frac{\partial \rho}{\partial x}+\rho\frac{\partial v_y}{\partial y}+v_y\frac{\partial \rho}{\partial y}+\rho\frac{\partial v_z}{\partial z}+v_z\frac{\partial \rho}{\partial z}\right]$$

Upon rearrangement, we get

$$\frac{\partial \rho}{\partial t}+v_x\frac{\partial \rho}{\partial x}+v_y\frac{\partial \rho}{\partial y}+v_z\frac{\partial \rho}{\partial z}=-\rho\left(\frac{\partial v_x}{\partial x}+\frac{\partial v_y}{\partial y}+\frac{\partial v_z}{\partial z}\right) \qquad (1.4.3\text{-}6)$$

This can be written using our definition of substantial derivative (Eq. 1.4.2-4) and vector notation as

$$\frac{D\rho}{Dt}=-\rho(\vec{\nabla}\,.\,\vec{v}) \qquad (1.4.3\text{-}7)$$

Equations 1.4.3-5 and 1.4.3-7 are useful forms of mass concentration in fluid systems and are forms of the ‘equation of continuity’ applicable to ‘continuum’ systems when the mean free path of the molecules (distance travelled by a molecule before colliding with another molecule) is less than a characteristic length.

When the density of a fluid can be assumed to be constant (fluid is incompressible), the LHS of the equations of continuity above go to zero. Thus, for an incompressible fluid, the equation of continuity simplifies to

$$(\vec{\nabla}\,.\,\vec{v})=0 \qquad (1.4.3\text{-}8)$$

Example 1.4.3-1

A design of a bioprocess device that is expected to handle a liquid presents the following flow in it. Check whether the design is feasible.

$$v_x = k_1(x^2 + y^2)$$
$$v_y = k_2(y^2 + z^2)$$
$$v_z = k_3(z^2 + x^2)$$

Solution

Since the flow equations need to satisfy the continuity equation (recall that the continuity equation represents mass conservation), it can be checked whether $(\vec{\nabla} \cdot \vec{v}) = 0$ for the above flow field. In an expanded representation, we need to check whether

$$\left(\frac{\partial}{\partial x} v_x + \frac{\partial}{\partial y} v_y + \frac{\partial}{\partial z} v_z \right) = 0$$

The LHS gives

$$2k_1x + 2k_2y + 2k_3z = 2(k_1x + k_2y + k_3z)$$

which is clearly not zero except at $k_1x + k_2y + k_3z = 0$. Thus, the design is feasible only on the plane $k_1x + k_2y + k_3z = 0$ which seems highly constrained and may not be suitable for a reasonably general application.

1.4.4 Equation of Continuity in Different Coordinate Systems

The equation of continuity was first presented in the rectangular coordinate system since the student can intuitively relate to it. In many situations, such as while dealing with cylindrical or spherical systems, the rectangular coordinate system becomes cumbersome to use. It is easier to use the relevant coordinate systems, and we need to know the equation of continuity in those systems. The equation of continuity in three commonly used coordinate systems is presented in Table 1.4.4-1. Some of the details of conversion from the rectangular coordinate system to other coordinate systems are given in Appendix 1.

Table 1.4.4-1 The equation of continuity

Rectangular coordinates

$$\frac{\partial\rho}{\partial t}+\left(\frac{\partial(\rho\, v_x)}{\partial x}+\frac{\partial(\rho\, v_y)}{\partial y}+\frac{\partial(\rho\, v_z)}{\partial z}\right)=0 \tag{A}$$

Cylindrical coordinates

$$\frac{\partial\rho}{\partial t}+\left(\frac{1}{r}\frac{\partial(\rho\, r\, v_r)}{\partial r}+\frac{1}{r}\frac{\partial(\rho\, v_\theta)}{\partial\theta}+\frac{\partial(\rho\, v_z)}{\partial z}\right)=0 \tag{B}$$

Spherical coordinates

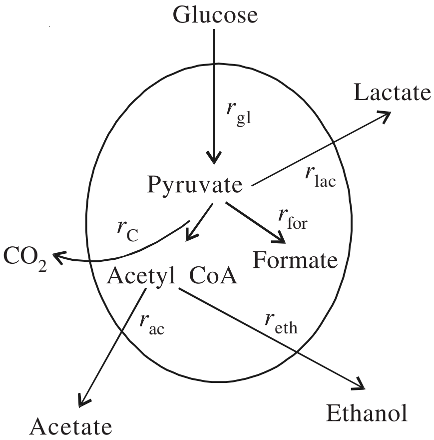
$$\frac{\partial\rho}{\partial t}+\left(\frac{1}{r^2}\frac{\partial(\rho\, r^2 v_r)}{\partial r}+\frac{1}{r\sin\theta}\frac{\partial(\rho\, v_\theta\sin\theta)}{\partial\theta}+\frac{1}{r\sin\theta}\frac{\partial(\rho\, v_\phi)}{\partial\phi}\right)=0 \tag{C}$$

Exercises

1. Succinctly distinguish between:
   (a) Continuum and discrete regimes
   (b) Total derivative and substantial derivative

2. What are the conditions under which the law of conservation of mass, Eq. 1.1.1-2, is valid?

3. Through suitable explicit material balances, express the relationships between the metabolites in the figure below in terms of the stoichiometric matrix, reaction rate and state vectors. Also in the case when the rates of lactate, ethanol, and glucose are available from measurements, estimate the rates of acetate, carbon dioxide, and formate in the system shown.



4. Develop the stoichiometric matrix, rate and state vectors for the following intracellular reaction scheme:

$$A \xrightarrow{r_1} B$$

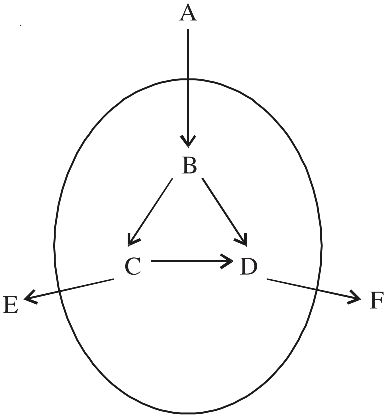
$$B \xrightarrow{r_2} 0.7\,C$$

$$B \xrightarrow{r_3} 0.5\,D$$

$$C \xrightarrow{r_4} 0.75\,D$$

$$C \xrightarrow{r_5} 0.9\,E$$

$$D \xrightarrow{r_6} 0.6\,F$$



5. An ineffective lecturer uses two chalk pieces to fill a black board of 1 m × 5 m. At the end of the class, the board is erased. The chalk piece can be considered cylindrical with a diameter of 1 cm and length, 7.5 cm. Each chalk piece weighs 3.5 g, and when discarded, its length is reduced to 2 cm. After the board is erased, what is the average area concentration of the chalk dust in g cm^{-2} in the vicinity of the board, which can be taken as 15 cm from the board. Assume that the dust taken away by the duster and the amount lost while writing consists of 85 % of the chalk used, and the remaining is present in the vicinity of the board.

6. In a milk processing plant, curd (yoghurt) is also manufactured. A continuous centrifuge needs to be used to produce buttermilk that contains less fat, and cream that contains high fat. If the average need is to process 48,000 kg of curd containing 4 % fat in an 8 hour shift, continuously, into a buttermilk stream that contains 0.5 % fat, and a cream stream with 50 % fat, what flow rates should the processing units for buttermilk and cream be equipped to handle, on an average?

7. During the studies for the liquid phase oxygen-supply strategy (LPOS) that was generalised in our laboratory, we performed two kinds of experiments – one, where the oxygen was supplied using only hydrogen peroxide pulses and two, where the oxygen was supplied using a combination of hydrogen peroxide pulses and aeration. Choose a suitable system, and write the various terms that would contribute to the mass balance on oxygen in the above two scenarios. (The means of finding the various terms would become clear only in the later chapters of this book.)

8. Even when only hydrogen peroxide pulses were used in the above problem on LPOS, since the bioreactor headspace was open to the atmosphere, albeit, aseptically through an outlet filter, the oxygen from the headspace would contribute to the balance. Modify the oxygen balance written above to include this aspect. Again, a way to determine the extent of the contribution is explained only in Chapter 6 of this text.

9. The flow through a bio-device that is being designed is given by the following expression

$$\vec{v} = k_1(-r^2)\hat{\imath}_r + k_2(r^2\theta)\hat{\imath}_\theta + k_3(2\,r\,z)\hat{\imath}_z$$

Check whether the design is feasible or not for an incompressible fluid.

10. Everyone in our hostels uses liquid mosquito repellents. A normal refill containing 35 ml of the repellent lasts for 45 nights (12 hours a night). Supposing a student switches it on at 19:00 h, what will be the concentration of the repellent in the room at 7:00 h, the next morning? Dimensions of the room are 1.5 × 2 × 3 m^3. Assume that the windows and doors are shut, and that the ceiling fan acts as a stirrer to maintain a uniform distribution of the repellent in the room.

11. Let us say that n_1 mmoles min^{-1} of air (assume that it contains only N_2 and O_2 in a 79:21 molar ratio) are inhaled and n_2 mmoles min^{-1} of a mixture of N_2, O_2, H_2O and CO_2 are exhaled during one cycle of respiration. Find n_1 and n_2, assuming that the energy is released gradually by oxidising 180 mg glucose min^{-1}. Also assume that 80 % of the oxygen inhaled is used for the oxidation of glucose, and the rest is exhaled; that the CO_2 arises only from glucose, and that 10 % of the water formed during respiration is exhaled.

12. Sometime after 2.5 mmoles of a drug are injected into the blood stream of a human being, its concentration becomes uniform in the blood. For effectiveness, the drug concentration in the blood needs to be above 100 mM, and below 500 mM to avoid side effects. When the blood flows through the kidney, 1 % of the drug is removed. The blood supply rate to the kidney is 1.5 l min^{-1}. Taking the total volume of blood in the human body to be 5 l, prescribe a dosage for the drug.

Some of the problems above were either suggested or formulated by G. Shashank, G. Vivek Sathvik, D. Divya Vani, I. Pradeep Kumar (5, 9–11), Shruthy Suresh, Purnima Padmanabhan (6), P. Raghavendran, P. Vivek, K. Ramasamy and M. Ashok (12).

Fully Open-ended Exercise

What is the ideal time gap between food intakes to prevent the stomach acid content from reaching unacceptable values?

(This exercise was formulated by Aparna B. Ganesh, for her CFA exercise – CFA stands for choose-focus-analyse. The details of the CFA exercise, and its goals are given in: Sureshkumar GK (2001) A Choose-Focus-Analyse Exercise in ChE Undergraduate Courses. Chemical Engineering Education 35: 80–84. Aparna's report can be found as a link from www.biotech.iitm.ac.in/GK_research.)

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Chapter 2
Mass Flux

In the previous chapter, we discussed the principle of mass balance and saw how it can be used in terms of mass or mass rates, to analyse, design and operate biosystems over a wide length scale, i.e. from a cell to a bioprocess. In this chapter, let us look at a concept that is central to many engineering disciplines, and especially to biological engineering, namely, flux.

A flux of a quantity is defined as the amount of that quantity that is transported per unit time across a unit area that is perpendicular to the direction of transport. Thus, mass flux is defined as the amount of mass transported per unit time across a unit area that is perpendicular to the direction of mass transport.

$$\text{Density} \times \text{Velocity} = \frac{\text{kg}}{\text{m}^3} \times \frac{\text{m}}{\text{s}} = \text{kg m}^{-2}\ \text{s}^{-1}$$

represents mass flux in appropriate (e.g. fluid) systems.

Mass flux is highly relevant in biological systems. The flux of glucose across a cell is essential for glycolysis to take place in many cells. The flux of a product (say ethanol) out of a cell is necessary to keep the cell alive as well as make the bioprocess viable. The transport of protein from the site of assembly to the site of function in a cell is essential for the viability of the cell. The mass flux of oxygen from the blood to the organ where the cells of the organ use the oxygen as the final electron acceptor is absolutely essential for the cells, thus, for the organ and ultimately for the animal/ human being to function well.

2.1 Primary Driving Force for Mass Flux

The primary driving force for mass flux is a difference in concentration of the substance being transported. To understand this better, let us imagine

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that a drop of ink is placed carefully, say using a pipette, inside (about halfway) a beaker containing water. The ink molecules will move away from the highly concentrated region i.e. where it was placed, to other parts of the beaker, until the concentration of ink in the beaker is uniform. The ink particles move because of the thermal energy of the molecules (ink and water molecules) that results in its random motion. In such cases, we say that diffusion of the species (ink) has occurred. Although the molecular motion due to thermal energy is random, the net movement of the species, or the ink flux in this case, is from a region of high ink concentration to a region of lower ink concentration.

The primary driving force being a concentration difference is only a first approximation, as students who understand thermodynamics would point out, which works well as long as we are restricted to fluxes in a single phase (gas, liquid, or solid) at dilute concentrations. The actual driving force is the difference in the chemical potential of the substance being transported. This works well in a single phase as well as across multiple phases.

Please note that we have used the term, ‘primary’ driving force. This is because mass flux can be caused by a variety of driving forces as we will see later in this chapter itself, and in a more structured fashion in Chapter 6. It so happens that concentration difference is ‘primarily’ or firstly linked to mass flux. However, we will encounter, even in this chapter, situations where mass flux (with respect to stationary coordinates) is caused by the entire fluid moving from one place to another. This is because the species constitute the fluid, and mass flux occurs when the fluid moves either due to application of a pressure gradient across a pipe, or because of gravity, or other factors. In other words, different driving forces cause mass flux, and concentration difference is considered the ‘primary’ driving force. Also, note that the primary driving force may not always cause the largest flux.

2.1.1 Basis for Expressing Mass Flux

Let us first consider the movement of a mixture containing various species. If v_i is the velocity of i^{th} species with respect to stationary coordinates axes, for a mixture of n species, the local mass average velocity $\vec{v}$ can be defined as

$$\vec{v} = \frac{\sum_{i=1}^{n} \rho_i \vec{v}_i}{\sum_{i=1}^{n} \rho_i} \qquad (2.1.1\text{-}1)$$

where ρ_i is the density of the i^{th} species.

Here we are not looking at velocities from the molecular point of view, but at the 'species' level. By 'species' level, the thinking is that we consider a group of molecules of the same species i in a tiny volume element, take the sum of their individual velocities and divide the sum by the number of such molecules in that tiny volume element.

Similar to the mass average velocity, a molar average velocity $\vec{v}^*$ can also be defined as

$$\vec{v}^* = \frac{\sum_{i=1}^{n} c_i \vec{v}_i}{\sum_{i=1}^{n} c_i} \tag{2.1.1-2}$$

where c_i is the concentration of species, i.

In a flowing system, the velocity of a species with respect to all species $\vec{v}$ or $\vec{v}^*$ is of more interest than the velocity with respect to stationary coordinates.

Thus, the useful quantities in such a system would be

$$\vec{v}_i - \vec{v} \ = \text{Diffusive velocity of } i \text{ with respect to } \vec{v} \tag{2.1.1-3}$$

and

$$\vec{v}_i - \vec{v}^* \ = \text{Diffusion velocity of } i \text{ with respect to } \vec{v}^* \tag{2.1.1-4}$$

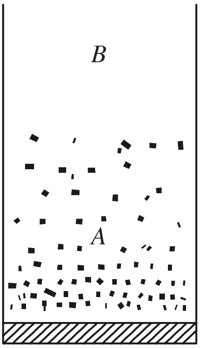
Example 2.1.1-1

To better understand the different velocities that we have just discussed, let us consider the disinfection of a lab using formaldehyde vapours. Typically, formalin solutions (~ 40 % w/v of formaldehyde in water) are used to generate formaldehyde vapours which can kill microorganisms in an enclosed space. Care is taken to seal all windows and doors with duct tape to prevent leakage of formaldehyde vapours when the disinfection is carried out. Potassium permanganate ($KMnO_4$) is added to formalin which results in an exothermic reaction. The increase in temperature causes the generation of formaldehyde vapours.

Let us assume that we are generating the formaldehyde vapours in a long cylinder (Fig. 2.1.1-1).

As can be imagined, at a particular time, the mole fraction of formaldehyde, x_A, will vary with the height in the cylinder. Let us consider the horizontal plane in the cylinder where $x_A = \frac{1}{5}$. Say that $\vec{v}^* = 7$ units at that plane and $\vec{v}_i - \vec{v}^* = 8$ units. Let us calculate the relevant velocities.

Fig. 2.1.1-1 The system considered here



A = Formaldehyde (HCHO) $M_A = 30$
B = Air $M_B = 29$

We know that $M_A = 30$ (HCHO) and $M_B = 29$ (air), and recognise that

$$\vec{v} = \frac{\sum_{i=1}^{n} \rho_i \vec{v}_i}{\sum_{i=1}^{n} \rho_i} = \frac{1}{(\rho_A + \rho_B)}(\rho_A \vec{v}_A + \rho_B \vec{v}_B) \tag{2.1.1-5}$$

Also, the mass fraction of A

$$w_A = \frac{m_A}{(m_A + m_B)} \tag{2.1.1-6}$$

If we divide both the numerator and the denominator of the RHS of Eq. 2.1.1-6 by V, we get

$$w_A = \frac{\rho_A}{\rho_A + \rho_B} \tag{2.1.1-7}$$

By using Eq. 2.1.1-7 in Eq. 2.1.1-5, and using a similar expression for w_B we get

$$\vec{v} = w_A \vec{v}_A + w_B \vec{v}_B \tag{2.1.1-8}$$

Also

$$\vec{v}^* = \frac{\sum_{i=1}^{n} c_i \vec{v}_i}{\sum_{i=1}^{n} c_i} = \frac{1}{(c_A + c_B)}(c_A \vec{v}_A + c_B \vec{v}_B) = x_A \vec{v}_A + x_B \vec{v}_B \tag{2.1.1-9}$$

where x = mole fraction.

Given that at the plane

$$x_A = \frac{1}{5}$$

$$\vec{v}^* = 7 \text{ units (upward direction is taken as positive)}$$

$$\vec{v}_A - \vec{v}^* = 8 \text{ units}$$

we can get

$$\vec{v}_A = 8 + \vec{v}^* = 15 \text{ units}$$

From $\vec{v}^* = x_A\vec{v}_A + x_B\vec{v}_B$, we get

$$7 = \frac{1}{5}(15) + \left(1 - \frac{1}{5}\right)\vec{v}_B$$

$$\therefore \quad \vec{v}_B = 5 \text{ units}$$

$$\therefore \quad \vec{v}_B - \vec{v}^* = -2 \text{ units (opposite direction)}$$

Now, we know that

$$w_A = \frac{m_A}{m_A + m_B} = \frac{x_A M_A}{x_A M_A + x_B M_B} = \frac{\frac{1}{5}\times 30}{\frac{1}{5}\times 30 + \frac{4}{5}\times 29} = \text{say, } 0.21$$

Therefore

$$w_B = 1 - 0.21 = 0.79$$

$$\vec{v} = w_A\vec{v}_A + w_B\vec{v}_B = 0.21\times 15 + 0.79\times 5 = 7.1 \text{ units}$$

and

$$\vec{v}_A - \vec{v} = 7.9 \text{ units}$$

$$\vec{v}_B - \vec{v} = -2.1 \text{ units (opposite direction)}$$

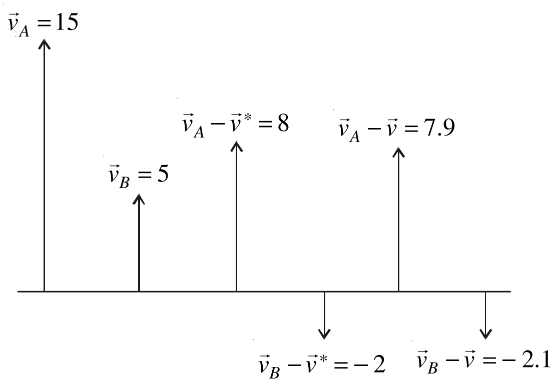
Figure 2.1.1-2 depicts the vartious velocities of formaldehyde and air in the cylinder.

2.1.2 Mass and Molar Fluxes

The mass flux of a species i with respect to stationary coordinates, as mentioned in the introductory part of this chapter, is

$$\vec{n}_i = \rho_i\vec{v}_i \quad \text{mass flux} \tag{2.1.2-1}$$

Fig. 2.1.1-2 Visualisation of the various velocities in the cylinder



Similarly, the molar flux can be written as

$$\vec{N}_i = c_i \vec{v}_i \quad \text{molar flux} \tag{2.1.2-2}$$

The mass (or molar) flux of a species *i* relative to mass average flux (with a mass average velocity $\vec{v}$) is

$$\vec{j}_i = \rho_i (\vec{v}_i - \vec{v}) \quad \text{mass flux} \tag{2.1.2-3}$$

$$\vec{J}_i = c_i (\vec{v}_i - \vec{v}) \quad \text{molar flux} \tag{2.1.2-4}$$

The mass (or molar) flux of a species *i* relative to molar average flux (with a molar average velocity $\vec{v}^*$) is

$$\vec{j}_i^* = \rho_i (\vec{v}_i - \vec{v}^*) \quad \text{mass flux} \tag{2.1.2-5}$$

$$\vec{J}_i^* = c_i (\vec{v}_i - \vec{v}^*) \quad \text{molar flux} \tag{2.1.2-6}$$

The fluxes $\vec{N}_i$, $\vec{j}_i$ and $\vec{J}_i^*$ are used more predominantly than the others, although there may be situations where the usage of other fluxes would be desirable.

Equation 2.1.2-6 can be written, using 2.1.1-2, as

$$\vec{J}_i^* = c_i v_i - \frac{c_i}{\sum_{j=1}^{n} c_j} \sum_{j=1}^{n} c_j \vec{v}_j$$

From Eq. 2.1.2-2, and the definition of mole fraction, the above equation can be written as

$$\vec{J}_i^* = \vec{N}_i - x_i \sum_{j=1}^{n} \vec{N}_j \tag{2.1.2-7}$$

or

$$\vec{J}_A^* = \vec{N}_A - x_A(\vec{N}_T) \tag{2.1.2-8}$$

where $\vec{N}_T = \vec{N}_A + \vec{N}_B$ for a binary system. Similarly, the mass flux can be written from Eq. 2.1.2-5 and 2.1.1-1, as

$$\vec{j}_i = \rho_i v_i - \frac{\rho_i}{\sum_{j=1}^{n} \rho_j} \sum_{j=1}^{n} \rho_j \vec{v}_j$$

From Eq. 2.1.2-1 and the definition of mass fraction, the above equation can be written as

$$\vec{j}_i = \vec{n}_i - w_i \sum_{j=1}^{n} \vec{n}_j \tag{2.1.2-9}$$

For a binary system

$$\vec{j}_A = \vec{n}_A - w_A(\vec{n}_A + \vec{n}_B) \tag{2.1.2-10}$$

Some useful relationships between the above velocities, fluxes, and mass (or mole) fractions, are covered in the exercises at the end of this chapter.

2.2 A Constitutive Equation

In the previous chapter, we discussed the representation of a general conservation principle, namely the mass conservation principle. The equation that represents such a principle is called the 'conservation equation' or the 'equation of change' which describes the system.

There exists a relationship between the flux of the conserved quantity and the material (constituent) properties of the system of interest. Such a relationship is not as generally applicable as the conservation equation, but is applicable to a class of similar substances. It is called a 'constitutive equation' or a 'constitutive relationship'.

Usually, a combination of constitutive equations (or equations of state) and the conservation equation (equation of change) are useful for the analysis and design of engineering systems.

2.2.1 Fick's First Law

The relationship between molar flux and concentrations in dilute binary solutions of non-reacting solutes was developed by Adolph Fick. It is known as Fick's I law. It can be represented in one dimension as

$$J_A^* = -D_{AB}\frac{dc_A}{dx} = -c\,D_{AB}\frac{dx_A}{dx} \qquad (2.2.1\text{-}1)$$

where D_{AB} is the mass diffusivity and it equals D_{BA}.

In the above equation, c is the total concentration, and x_A is the mole fraction of A. Thus, the species A moves relative to the mixture in the direction of the decreasing mole fraction of A. The derivation of Fick's I law is given in Appendix 2.

Of greater importance, note that Eq. 2.2.1-1 says that mass flux is proportional to the negative of the concentration gradient. In general, *any flux is proportional to the negative of a certain gradient*. This *gradient* is that of the *primary driving force* for that particular *flux*. In this case, the mass flux is proportional to the gradient of its primary driving force, i.e. concentration difference.

In three dimensions, Fick's I law can be represented as

$$\vec{J}_A^* = -c\,D_{AB}\vec{\nabla}x_A \qquad (2.2.1\text{-}2)$$

There are various methods to estimate D_{AB} and its dependence on pressure and temperature. The interested reader can find these methods in books such as *Transport Phenomena* by Bird et al. (2002).

Although the remainder of this section better belongs in Chapter 6, because there are two driving forces for mass transport (concentration difference and convection through bulk flow), for completeness, especially of a subsequent material balance aspect in this chapter, let us consider it here.

Upon substitution of Eq. 2.2.1-2 in Eq. 2.1.2-8, we get

$$-c\,D_{AB}\vec{\nabla}x_A = \vec{N}_A - x_A(\vec{N}_T) \qquad (2.2.1\text{-}3)$$

or

$$\underset{\text{(Diffusion)}}{\vec{N}_A = -c\,D_{AB}\vec{\nabla}x_A} \quad + \quad \underset{\text{(Bulk motion)}}{x_A(\vec{N}_T)} \qquad (2.2.1\text{-}4)$$

where $\vec{N}_T = \vec{N}_A + \vec{N}_B$ for a binary system. Eq. 2.2.1-4 shows that the flux $\vec{N}_A$, relative to stationary coordinates, is the resultant of two vector quantities

$x_A(\vec{N}_T)$ = Molar flux of A resulting from the bulk motion of the liquid

and

$-c\,D_{AB}\vec{\nabla}x_A = \vec{J}_A^*$ = Molar flux of A resulting from the diffusion superimposed on the bulk flow

In terms of mass, Fick's first law can be written as

$$\vec{j}_A = -\rho D_{AB} \vec{\nabla} w_A \tag{2.2.1-5}$$

The D_{AB} is the same as in Eq. 2.2.1-2.

Substituting Eq. 2.2.1-5 in Eq 2.1.2-10, we get

$$-\rho D_{AB} \vec{\nabla} w_A = \vec{n}_A - w_A(\vec{n}_T) \tag{2.2.1-6}$$

where $\vec{n}_T = \vec{n}_A + \vec{n}_B$ for a binary system.

2.2.1.1 In Concentrated Solutions

In dilute solutions, the solute-solute interactions can be ignored, whereas in concentrated solutions, they cannot be ignored. In such a case, the driving force for mass flux is not the concentration gradient, but the gradient in chemical potential, μ_A, as may be known from thermodynamics.

$$\vec{J}_A^* = -\frac{c_A}{RT} D_{AB} \frac{d\mu_A}{dz} \tag{2.2.1.1-1}$$

The above equation can be expressed in terms of the easily measurable concentration, rather than in terms of the difficult to measure, chemical potential, as below

$$\vec{J}_A^* = -D_{\text{eff}} \frac{dc_A}{dz} \tag{2.2.1.1-2}$$

where

$$D_{\text{eff}} = D_{AB} \left[\frac{d \ln \gamma_A}{d \ln x_A} + 1 \right] \tag{2.2.1.1-3}$$

where γ_A is the activity coefficient of A.

The derivation of the above equation is given in Appendix 3. Nevertheless, the above equation has limitations because the activity coefficients of many solutes as a function of their composition are unknown.

2.3 Solution Approaches

Diffusion is highly relevant in biological systems. The function of a cell is determined by the diffusion of various substances through the cell membrane. Diffusion of a drug molecule from the blood stream to the site of action determines the efficacy of the drug, and so on.

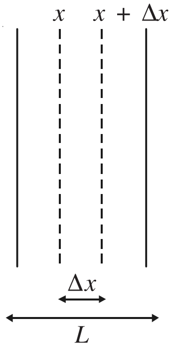


Fig. 2.3.1-1 The 'shell' considered for the analysis

To begin with, let us consider one-dimensional diffusion across a uniform material. Broadly, there are two approaches to solve relevant problems: (i) the shell balance approach, and (ii) the application of the relevant conservation equation, i.e. the equation of continuity in this case of mass conservation.

2.3.1 Shell Balance Approach

Let us consider a material, say a uniform membrane. In this membrane, let us consider a *shell* of thickness Δx through which diffusion occurs normal to the surface area A in the direction perpendicular to the page (Fig. 2.3.1-1); L is the thickness of the membrane. The shell will represent the geometry under consideration. In this case, the shell is a cuboid; in the case of cylindrical systems, it could be an annular cylinder, and in the case of spherical coordinates, it could be an annular sphere. Since we balance over a shell, this approach is called a 'shell balance' approach.

A material balance written over the shell (system) on component i entering at x and leaving at $x + \Delta x$ in terms of molar flux, following the approach presented in Chapter 1, yields

$$\frac{dA_i}{dt} = \dot{I}_i - \dot{O}_i + \dot{G}_i - \dot{C}_i$$

$$\frac{\partial c_i}{\partial t} A\,\Delta x = N_i\,|_x\, A - N_i\,|_{x+\Delta x}\, A + R_i\, A\,\Delta x \tag{2.3.1-1}$$

Dividing each term by the volume element, $A\,\Delta x$ gives

$$\frac{\partial c_i}{\partial t} = \frac{N_i\,|_x - N_i\,|_{x+\Delta x}}{\Delta x} + R_i$$

If we employ the limit $\Delta x \to 0$, and use the definition of the derivative

$$\frac{\partial c_i}{\partial t} = -\frac{\partial N_i}{\partial x} + R_i \tag{2.3.1-2}$$

In this case, the flux N_i results only from diffusion. Thus

$$\vec{N}_i = \vec{J}_i^* = -D_i \frac{\partial c_i}{\partial x}$$

Therefore

$$\frac{\partial c_i}{\partial t} = D_i \frac{\partial^2 c_i}{\partial x^2} + R_i \tag{2.3.1-3}$$

When there is no production of i in the volume, $A\,\Delta x$, say by a reaction, then

$$\frac{\partial c_i}{\partial t} = D_i \frac{\partial^2 c_i}{\partial x^2} \tag{2.3.1-4}$$

The above Eq. 2.3.1-4 is known as Fick's second law.

Under steady state conditions (no time dependence i.e. concentration does not vary with time), the LHS of Eq. 2.3.1-4 becomes zero. Thus

$$0 = D_i \frac{\partial^2 c_i}{\partial x^2} \tag{2.3.1-5}$$

Equation 2.3.1-5 is the one-dimensional diffusion equation under steady state conditions with no reaction.

In three dimensions, under the same conditions, Fick's second law can be written as

$$\frac{\partial c_i}{\partial t} = 0 = D_i\, \nabla^2 c_i \tag{2.3.1-6}$$

2.3.2 Continuity (Conservation) Equation Approach

The same result obtained in Eq. 2.3.1-5 can be derived by applying the material/mass balance equation directly over the relevant system. The shell balance approach provides an intuitive mechanistic appreciation of the process for the inexperienced reader, but it could become cumbersome if the situation is not simple enough. In most cases, the material balance equation approach is easier to use, although it may seem more abstract to a not so experienced reader.

In any case, we first need to derive the useful material balance equation for binary/multi-component systems. This is because the mass balance equations that we had developed in Chapter 1, i.e.

$$\frac{\partial \rho}{\partial t} = -(\vec{\nabla}.\rho\vec{v}) \tag{1.4.3-5}$$

and

$$\frac{D\rho}{Dt} = -\rho(\vec{\nabla}\,.\,\vec{v}) \tag{1.4.3-7}$$

are applicable only to a single component system or to the total mass in a multi-component system.

Let us first consider a multi-component mixture. Let us take a cuboidal element, $\Delta x\Delta y\Delta z$, fixed in space (same as in Fig. 1.4.3-1) through which the multi-component mixture is flowing.

Let us apply the mass conservation principle to A, which is a species in the multi-component mixture. Recall that

$$\frac{dA}{dt} = \dot{I} - \dot{O} + \dot{P} \tag{1.4.3-1}$$

Thus

$$\frac{\partial A}{\partial t} = \frac{\partial \rho_A}{\partial t}\Delta x\Delta y\Delta z$$

$$\dot{I}\,|_x = (n_{Ax})\,|_x\;\Delta y\Delta z$$

$$\dot{I}\,|_y = (n_{Ay})\,|_y\;\Delta x\Delta z$$

$$\dot{I}\,|_z = (n_{Az})\,|_z\;\Delta x\Delta y$$

$$\dot{O}\,|_{x+\Delta x} = (n_{Ax})\,|_{x+\Delta x}\;\Delta y\Delta z$$

$$\dot{O}\,|_{y+\Delta y} = (n_{Ay})\,|_{y+\Delta y}\;\Delta x\Delta z$$

$$\dot{O}\,|_{z+\Delta z} = (n_{Az})\,|_{z+\Delta z}\;\Delta x\Delta y$$

$$\dot{P} = r_A\Delta x\Delta y\Delta z$$

Substituting the terms in Eq. 1.4.3-1, dividing throughout by the volume element $\Delta x\Delta y\Delta z$, and taking the limit as $\Delta x \to 0$, $\Delta y \to 0$, $\Delta z \to 0$, we get

$$\frac{\partial \rho_A}{\partial t} + \left(\frac{\partial n_{Ax}}{\partial x} + \frac{\partial n_{Ay}}{\partial y} + \frac{\partial n_{Az}}{\partial z}\right) = r_A \tag{2.3.2-1}$$

In a compact form

$$\frac{\partial \rho_A}{\partial t} + (\vec{\nabla}\,.\,\vec{n}_A) = r_A \tag{2.3.2-2}$$

Note that $\vec{n}_A = \rho_A\vec{v}_A$.

Equation 2.3.2-2 is the equation of continuity for component A in a multi-component mixture.

Suppose the mixture is binary with only components A and B. We can derive the equation of continuity for component B as

$$\frac{\partial \rho_B}{\partial t} + (\vec{\nabla} \,.\, \vec{n}_B) = r_B \qquad (2.3.2\text{-}3)$$

For a binary mixture, since $\vec{n}_A + \vec{n}_B = \rho\vec{v}$, $\vec{\rho}_A + \vec{\rho}_B = \rho$ and $r_A + r_B = 0$ (recall the definition of r_A and r_B; in a binary system, $r_A = -r_B$), the addition of Eq. 2.3.2-2 and Eq. 2.3.2-3 yields

$$\frac{\partial \rho}{\partial t} + (\vec{\nabla} \,.\, \rho\vec{v}) = 0$$

our earlier total mass balance equation.

Moreover, if the density is constant

$$(\vec{\nabla} \,.\, \vec{v}) = 0$$

which is the equation of continuity for the total mass balance with constant density.

If we had used molar units instead of mass units, the extent of general applicability would be compromised because moles are conserved under more stringent conditions than is mass. However, in many situations, molar units are convenient. In terms of moles, the Eqs. 2.3.2-2 and 2.3.2-3 would have been

$$\frac{\partial c_A}{\partial t} + (\vec{\nabla} \,.\, \vec{N}_A) = R_A \qquad (2.3.2\text{-}4)$$

and

$$\frac{\partial c_B}{\partial t} + (\vec{\nabla} \,.\, \vec{N}_B) = R_B \qquad (2.3.2\text{-}5)$$

Adding the above equations with the realisation that $c_A + c_B = c$ and $\vec{N}_A + \vec{N}_B = c\vec{v}^*$ and $R_A + R_B \neq 0$ unless one mole of A produces/results from one mole of B, we obtain

$$\frac{\partial c}{\partial t} + (\vec{\nabla} \,.\, c\vec{v}^*) = R_A + R_B \qquad (2.3.2\text{-}6)$$

and for constant c

$$(\vec{\nabla} \,.\, \vec{v}^*) = \frac{1}{c}(R_A + R_B) \qquad (2.3.2\text{-}7)$$

If we replace $\vec{n}_A$ and $\vec{N}_A$ in Eq. 2.3.2-2 and Eq. 2.3.2-4 in terms of descriptive equations, we can get more useful relations.

Let us substitute Eq. 2.2.1-4 in Eq. 2.3.2-4

$$\frac{\partial c_A}{\partial t} + \left(\vec{\nabla} \cdot \left[-cD_{AB}\vec{\nabla}x_A + x_A(\vec{N}_A + \vec{N}_B)\right]\right) = R_A$$

or

$$\frac{\partial c_A}{\partial t} + \left(\vec{\nabla} \cdot [-cD_{AB}\vec{\nabla}x_A + x_A c\vec{v}^*]\right) = R_A$$

i.e.

$$\frac{\partial c_A}{\partial t} + \vec{\nabla} \cdot c_A\vec{v}^* = (\vec{\nabla} \cdot cD_{AB}\vec{\nabla}x_A) + R_A \tag{2.3.2-8}$$

Similarly, let us substitute Eq. 2.2.1-6 in Eq. 2.3.2-2; we get

$$\frac{\partial \rho_A}{\partial t} + \left(\vec{\nabla} \cdot \left[-\rho D_{AB}\vec{\nabla}w_A + w_A(\vec{n}_A + \vec{n}_B)\right]\right) = r_A$$

i.e.

$$\frac{\partial \rho_A}{\partial t} + \vec{\nabla} \cdot \rho_A\vec{v} = (\vec{\nabla} \cdot \rho D_{AB}\vec{\nabla}w_A) + r_A \tag{2.3.2-9}$$

When c and D_{AB} are constant Eq. 2.3.2-8 can be expressed as

$$\frac{\partial c_A}{\partial t} + c_A(\vec{\nabla} \cdot \vec{v}^*) + (\vec{v}^* \cdot \vec{\nabla}c_A) = D_{AB}\vec{\nabla}^2 c_A + R_A$$

or

$$\frac{\partial c_A}{\partial t} + (\vec{v}^* \cdot \vec{\nabla}c_A) = D_{AB}\vec{\nabla}^2 c_A + R_A - \frac{c_A}{c}(R_A + R_B) \tag{2.3.2-10}$$

because $\vec{\nabla} \cdot \vec{v}^* = \frac{1}{c}(R_A + R_B)$ from Eq. 2.3.2-7.

Similarly, when ρ and D_{AB} are constant (for example, ρ is almost constant in liquid systems when there is no significant change in temperature; constant D_{AB} is a good assumption in many dilute systems), Eq. 2.3.2-9 can be expressed as

$$\frac{\partial \rho_A}{\partial t} + \rho_A(\vec{\nabla} \cdot \vec{v}) + (\vec{v} \cdot \vec{\nabla}\rho_A) = D_{AB}\vec{\nabla}^2 \rho_A + r_A$$

or

$$\frac{\partial \rho_A}{\partial t} + (\vec{v} \cdot \vec{\nabla}\rho_A) = D_{AB}\vec{\nabla}^2 \rho_A + r_A \tag{2.3.2-11}$$

since $\vec{\nabla} \cdot \vec{v} = 0$.

If we divide throughout by M_A, the molecular mass of A, we get

$$\frac{\partial c_A}{\partial t} + (\vec{v} \,.\, \vec{\nabla} c_A) = D_{AB} \vec{\nabla}^2 c_A + R_A \qquad (2.3.2\text{-}12)$$

For a multi-component system, one needs to invoke the Maxwell-Stefan equations to appropriately derive the relevant expressions (Bird et al. 2002). Let us use the earlier approach for a single component system as it is fairly simple. Substituting Eq. 2.2.1-2 in the relevant form of Eq. 2.1.2-7 we get

$$N_A = -\, c\, D_{AB} \vec{\nabla} x_A + x_A (\Sigma_i \vec{N}_i)$$

Substitution of the above equation in Eq. 2.3.2-4 yields

$$\frac{\partial c_A}{\partial t} + \left(\vec{\nabla} \,.\left[-\, c\, D_{AB} \vec{\nabla} x_A + x_A (\Sigma_i \vec{N}_i)\right]\right) = R_A$$

which results in the same equation 2.3.2-8 since now, $\Sigma_i \vec{N}_i = c\, \vec{v}^*$.

Through extension of the above argument for the mass basis, we can see that Eq. 2.3.2-12 is valid for multi-component systems.

This equation can be used to get concentration profiles. The forms of the equation in various coordinate systems are given in Table 2.3.2-1. Please note that since the equations have been derived on a molar basis, it is difficult to apply them in a flow system with changing cross-sectional area; when the cross-sectional area changes, molar concentrations vary. However, they are useful in many situations of practical interest (where the cross-sectional area does not change).

Example 2.3.2-1

Let us get back to the first sentence of this section. We can derive Eq. 2.3.1-5 by applying the material/mass balance equation directly over the relevant system. The system here is the membrane through which diffusion occurs. Since the problem deals with a one-dimensional motion and steady state, let us consider the relevant terms in equation A2 (Table 2.3.2-1), since ρ and D_{AB} can be considered constant here (A is the species and B is the membrane material). Some of the terms in the equation can also be equated to zero; the reasons are given below (SS refers to steady state, and *rxn* refers to reaction).

Here, since the analysis is being done at SS, the time derivative is zero; since there is no bulk flow, the velocity components v_x, v_y and v_z are zero; since the concentration does not vary in the y and z directions, the corresponding (first and second) derivatives are zero; and since there is no reaction taking place, the reaction rate is zero.

Table 2.3.2-1 The equation of continuity of a species, say *A*, in a multi-component mixture in various coordinate systems

---

Rectangular coordinates

$$\frac{\partial c_A}{\partial t}+\left(\frac{\partial N_{Ax}}{\partial x}+\frac{\partial N_{Ay}}{\partial y}+\frac{\partial N_{Az}}{\partial z}\right)=R_A \tag{A1}$$

When c and D_{AB} are constant

$$\frac{\partial c_A}{\partial t}+\left(v_x\frac{\partial c_A}{\partial x}+v_y\frac{\partial c_A}{\partial y}+v_z\frac{\partial c_A}{\partial z}\right)-D_{AB}\left(\frac{\partial^2 c_A}{\partial x^2}+\frac{\partial^2 c_A}{\partial y^2}+\frac{\partial^2 c_A}{\partial z^2}\right)=R_A \tag{A2}$$

Cylindrical coordinates

$$\frac{\partial c_A}{\partial t}+\left(\frac{1}{r}\frac{\partial}{\partial r}(rN_{Ar})+\frac{1}{r}\frac{\partial N_{A\theta}}{\partial \theta}+\frac{\partial N_{Az}}{\partial z}\right)=R_A \tag{B1}$$

When c and D_{AB} are constant

$$\begin{aligned}&\frac{\partial c_A}{\partial t}+\left(v_r\frac{\partial c_A}{\partial r}+v_\theta\frac{1}{r}\frac{\partial c_A}{\partial \theta}+v_z\frac{\partial c_A}{\partial z}\right)\\&-D_{AB}\left(\frac{1}{r}\frac{\partial}{\partial r}\left(r\frac{\partial c_A}{\partial r}\right)+\frac{1}{r^2}\frac{\partial^2 c_A}{\partial \theta^2}+\frac{\partial^2 c_A}{\partial z^2}\right)=R_A\end{aligned} \tag{B2}$$

Spherical coordinates

$$\frac{\partial c_A}{\partial t}+\left(\frac{1}{r^2}\frac{\partial}{\partial r}(r^2N_{Ar})+\frac{1}{r\sin\theta}\frac{\partial}{\partial \theta}(N_{A\theta}\sin\theta)+\frac{1}{r\sin\theta}\frac{\partial N_{A\phi}}{\partial \phi}\right)=R_A \tag{C1}$$

When c and D_{AB} are constant

$$\begin{aligned}&\frac{\partial c_A}{\partial t}+\left(v_r\frac{\partial c_A}{\partial r}+v_\theta\frac{1}{r}\frac{\partial c_A}{\partial \theta}+v_\phi\frac{1}{r\sin\theta}\frac{\partial c_A}{\partial \phi}\right)\\&-D_{AB}\left(\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial c_A}{\partial r}\right)+\frac{1}{r^2\sin\theta}\frac{\partial}{\partial \theta}\left(\sin\theta\frac{\partial c_A}{\partial \theta}\right)+\frac{1}{r^2\sin^2\theta}\frac{\partial^2 c_A}{\partial \phi^2}\right)=R_A\end{aligned} \tag{C2}$$

$$\overset{= 0\ (\text{SS})}{\cancel{\frac{\partial c_A}{\partial t}}} + \left(v_x \overset{= 0\ (v_x = 0)}{\cancel{\frac{\partial c_A}{\partial x}}} + v_y \overset{= 0\ (v_y = 0)}{\cancel{\frac{\partial c_A}{\partial y}}} + v_z \overset{= 0\ (v_z = 0)}{\cancel{\frac{\partial c_A}{\partial z}}} \right) - D_{AB} \left(\frac{\partial^2 c_A}{\partial x^2} + \overset{= 0\ (c_A \neq f(y))}{\cancel{\frac{\partial^2 c_A}{\partial y^2}}} + \overset{= 0\ (c_A \neq f(z))}{\cancel{\frac{\partial^2 c_A}{\partial z^2}}} \right) = \overset{= 0\ (\text{no } rxn)}{\cancel{R_A}}$$

Hence
$$D_{AB} \frac{\partial^2 C_A}{\partial x^2} = 0$$

which is the same equation as earlier (Eq. 2.3.1-5) that has been arrived at without the shell balance. As mentioned earlier, in many cases, shell balances are cumbersome, and direct application of the continuity equation is preferred once the system and its boundaries over which it is applied is clear.

2.4 Steady State Diffusion

Steady state, as briefly mentioned in the previous section, refers to the condition when the properties of interest at a point in space do not change with time, i.e. are not functions of time, and thus the time derivatives can be set to zero. Many real biological diffusion cases can be approximated to steady state diffusion in one dimension across a ‘lumped’ uniform membrane. For example, when concentrations are uniform over a surface, the curvature is not significant, and the thickness is very less compared to the length or breadth, the above approximation holds; using this approximation, the diffusion across the surfaces of tissues or large organs such as the skin or the kidney can be considered as a steady state diffusion.

2.4.1 Steady State Diffusion Across Membranes

There are two broad ways in which diffusion across a membrane can be viewed

(i) Dissolve-diffuse mechanism: The solute first dissolves in the membrane and then diffuses through it.
(ii) Diffusion through pores: The solute moves through pores in the membrane material which is otherwise impermeable to the solute.

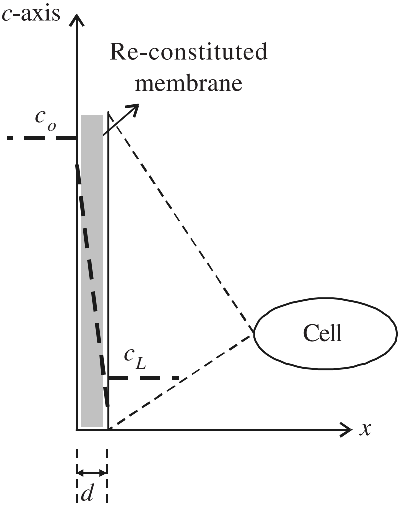


Fig. 2.4.1-1 The cell membrane considered here; the membrane curvature is neglected

Dissolve-Diffuse Mechanism

A species i diffuses across a membrane of thickness d through the dissolve-diffuse mechanism (Fig. 2.4.1-1). The concentration of i outside the cell is c_o and that inside the cell is c_L.

At $x = 0$, the concentration of i in the membrane is given by Kc_o, where K is the partition coefficient of i in the membrane. Partition coefficient is defined as the ratio of the solute concentrations in two phases at equilibrium, when a solute is partitioning across the two phases.

$$c_m|_{x=0} = Kc_o$$

and

$$c_m|_{x=d} = Kc_L$$

We have assumed that the partition coefficient is the same on both sides of the membrane. This is a reasonable assumption, but may not be applicable in situations where solutions on both sides of the membrane are widely different.

Example 2.4.1-1

Develop an expression for the flux of species i across a membrane by assuming a dissolve-diffuse mechanism.

Solution

Note that Eq. 2.3.1-5 is applicable here (why? – note that steady state conditions prevail in the system). But, since diffusion is through a complex membrane, an effective diffusive coefficient $D_{i,\text{eff}}$ needs to be used. Further, since the variation is only with one variable (the dimension), the partial derivative can be replaced by a total derivative.

$$0 = D_{i,\text{eff}} \frac{d^2 c_m}{d x^2} \tag{2.4.1-1}$$

The boundary conditions are:

At $x = 0,\ c_m = Kc_o$ (2.4.1-2)

$x = d,\ c_m = Kc_L$ (2.4.1-3)

where K is the partition coefficient defined as the ratio of the species concentration in the membrane to that in the bulk solution.

The solution obtained by integrating Eq. 2.4.1-1 twice with the realisation that the second derivative is zero, and hence, the first derivative is a constant is

$$c_m = C_1 x + C_2 \tag{2.4.1-4}$$

where C_1 and C_2 are constants that can be evaluated using boundary conditions. At $x = 0$

$$C_2 = Kc_o \tag{2.4.1-5}$$

At $x = d$

$$Kc_L = C_1 d + Kc_o$$

Therefore

$$C_1 = \frac{-K(c_o - c_L)}{d} \tag{2.4.1-6}$$

Now, by substituting Eq. 2.4.1-5 and Eq. 2.4.1-6 in Eq. 2.4.1-4 we get

$$c_m = Kc_o - K(c_o - c_L)\frac{x}{d} \tag{2.4.1-7}$$

Thus

$$\vec{J}_i^* = -D_{i,\text{eff}} \frac{\partial c_m}{\partial x} = \frac{K D_{i,\text{eff}}}{d}(c_o - c_L) \tag{2.4.1-8}$$

Comment

Since this is a steady state process, the flux is a constant, and as the equation indicates, it is independent of position.

If $c_o > c_L$ the flux is in the positive x direction.
If $c_o < c_L$ the flux is in the negative x direction.
$\dfrac{K D_{i,\mathrm{eff}}}{d}$ is defined as 'permeability' P of the solute i across the membrane.

Note that it is a product of the partition coefficient K and diffusivity $D_{i,\mathrm{eff}}$. The dependence of permeability on both the above parameters indicates the dissolve (K)-diffuse ($D_{i,\mathrm{eff}}$) mechanism. Nevertheless, permeability is not an intrinsic membrane property since it depends on the thickness of the membrane, d.

Also, note that

$$K = \frac{c_m|_{x=0}}{c_o}$$

and we have assumed that to be equal to

$$\frac{c_m|_{x=d}}{c_L}$$

If $K < 1$, $c_m|_{x=0} < c_o$ and $c_m|_{x=d} < c_L$.

In other words, the concentrations on the membrane surfaces are less than those in the fluids. Notice the dark-dotted line and the discontinuities at the surface that represents the species concentration in Fig. 2.4.1-1.

Diffusion through Pores in a Membrane

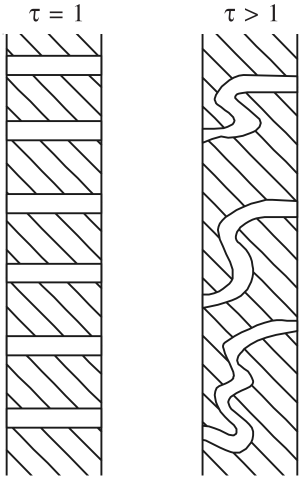
Let us consider a membrane made up of pores in an impermeant matrix – a matrix through which solutes cannot dissolve and diffuse. The pores, however, are filled with a solvent through which the solute diffuses.

When the Pores are Large
When the dimension of the pores are much larger than the solute size, the permeability can be modified as

$$P' = \left(\frac{D_i K}{d}\right)\left(\frac{\epsilon}{\tau}\right)$$

where D_i is diffusivity of solute i in free solution, K is partition coefficient of the solute between the solvent in bulk and the solvent in the pores; it can usually be approximated that the concentration of the solute in bulk and the

Fig. 2.4.1-2 Different tortuosities that are possible in membranes



solute in the solvent are the same and hence $K = 1$ is a good approximation, d is membrane thickness, τ is tortuosity (Fig. 2.4.1-2), a measure of the mean distance travelled by the solute in relation to the thickness of the membrane and

ε = Porosity = Volume fraction of pores in the membrane

$$= \frac{\text{Volume of pores}}{\text{Total volume of the membrane including pores}}$$

When the Pores are Comparable in Size to the Solute

When the pores become sufficiently small, the diffusivity in a pore is less than that in free solution. This process is sometimes referred to as hindered diffusion. We give the final expression for the modified permeability in such a case. The derivation can be found in other sources (e.g. Weiss 1996)

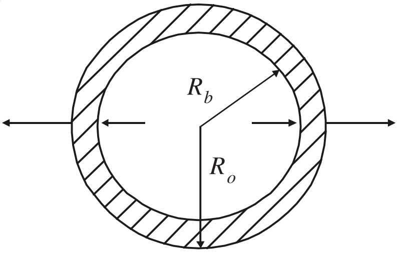
$$P'' = \frac{\left[D_i F\left(\frac{a}{r}\right)\right]}{d \quad \tau} K \left\{ \left(1 - \frac{a}{r}\right)^2 \right\} \varepsilon$$

where $F\left(\frac{a}{r}\right) \simeq 1 - 2.1044\left(\frac{a}{r}\right) + 2.089\left(\frac{a}{r}\right)^3 - 0.948\left(\frac{a}{r}\right)^5$ for $\left(\frac{a}{r}\right) < 0.4$

r is pore radius and a is solute radius.

The factor $D_i F\left(\frac{a}{r}\right)$ accounts for the modified diffusivity due to the small pore size (hydrodynamic hindrance). The factor $K\left(1 - \frac{a}{r}\right)^2$ accounts

Fig. 2.4.2-1 The cross-section of the bronchiole



for the modified partitioning of the solute between the solution and the pore (stearic hindrance).

2.4.2 Steady State Radial Diffusion Across Tubular Walls

There exist many examples of tubular elements in biological systems. For example, our vascular system (arteries, veins, etc.) are all tubular elements, to a first approximation. So are the air passages that lead to the lungs.

Example 2.4.2-1

In certain conditions of respiratory difficulty, a drug is administered continuously through the nasal cavity, at an appropriate dose, to reach the lung tissue by passing across the bronchiole wall. The concentration of the drug in the air present in the lumen of the bronchiole is c_b at steady state. The drug concentration in the lung tissue on the other side of the bronchiolar wall is needed to be c_o for effectiveness. The inner and outer radii of the bronchiole are R_b and R_o, respectively (Fig. 2.4.2-1). Let us study this process to get an expression for the radial drug flux at the inner wall of the bronchiole that is needed to ensure effectiveness of the drug. Assume that at the region of analysis, the difference in the drug concentration in the z direction on the bronchiole wall can be neglected.

Since we are studying a cylindrical system, it will be easier to employ cylindrical coordinates.

Let us consider the bronchiole wall as our system, the drug as the species of interest, and then do a mass balance of the species on our system. We can directly use the equation of continuity in cylindrical coordinates.

Consider Eq. B2 from Table 2.3.2-1

$$\overset{=0\ (\text{SS})}{\cancel{\frac{\partial c_A}{\partial t}}} + \left(\overset{=0\ (v_r=0)}{\cancel{v_r}} \frac{\partial c_A}{\partial r} + \overset{=0\ (v_\theta=0)}{\cancel{v_\theta}} \frac{1}{r}\frac{\partial c_A}{\partial \theta} + v_z \overset{=0\ (c_A \neq f(z))}{\cancel{\frac{\partial c_A}{\partial z}}}\right) - D_{AB}\left(\frac{1}{r}\frac{\partial}{\partial r}\left(r\frac{\partial c_A}{\partial r}\right) + \overset{=0\ (c_A \neq f(\theta))}{\cancel{\frac{1}{r^2}\frac{\partial^2 c_A}{\partial \theta^2}}} + \overset{=0\ (c_A \neq f(z))}{\cancel{\frac{\partial^2 c_A}{\partial z^2}}}\right) = \overset{=0\ (\text{no } rxn)}{\cancel{R_A}}$$

Hence

$$D_{AB}\left(\frac{1}{r}\frac{\partial}{\partial r}\left(r\frac{\partial C_A}{\partial r}\right)\right) = 0$$

Since r is the only independent variable here, we can replace the partial derivatives with total derivatives. Thus

$$D_{AB}\left(\frac{1}{r}\frac{d}{dr}\left(r\frac{dC_A}{dr}\right)\right) = 0 \qquad (2.4.2\text{-}1)$$

The boundary conditions are

$$c_A = Kc_b \text{ at } r = R_b \qquad (2.4.2\text{-}2)$$

$$c_A = Kc_o \text{ at } r = R_o \qquad (2.4.2\text{-}3)$$

where K is the distribution coefficient, i.e. the ratio of the drug concentrations in the two phases at equilibrium. For Eq. 2.4.2-2, the phases are the air inside the bronchiole and the bronchiole wall. For Eq. 2.4.2-3 the phases are the air outside the bronchiole and the bronchiole wall.

On solving Eq. 2.4.2-1 (note that for the derivative in the equation to be zero, $r\frac{dC_A}{dr}$ = constant, say C_1), we get

$$c_A = C_1 \ln r + C_2 \qquad (2.4.2\text{-}4)$$

Using the boundary conditions, we can get

$$C_1 = \frac{K(c_b - c_o)}{\ln\left(\frac{R_b}{R_o}\right)}$$

$$C_2 = Kc_b - K(c_b - c_o)\frac{\ln(R_b)}{\ln\left(\frac{R_b}{R_o}\right)}$$

Substituting C_1 and C_2 in Eq. 2.4.2-4 and rearranging, we get

$$C_A = KC_b - K(C_b - C_o)\frac{\ln\left(\frac{R_b}{r}\right)}{\ln\left(\frac{R_b}{R_o}\right)} \tag{2.4.2-5}$$

Thus, the flux at R_b

$$\vec{J}_A^* = -D_{AB}\left.\frac{\partial C_A}{\partial r}\right|_{r=R_b} = \left.\frac{D_{AB}K(C_b - C_o)}{r\ln\left(\frac{R_b}{R_o}\right)}\right|_{r=R_b} = \frac{D_{AB}K(C_b - C_o)}{R_b\ln\left(\frac{R_b}{R_o}\right)} \tag{2.4.2-6}$$

2.4.3 Steady State Radial Diffusion Across Spherical Pellets

To illustrate how the mass balance/continuity equation can be used to get important parameters in a system that is easiest analysed using a spherical coordinate system, let us consider an example.

Example 2.4.3-1

To improve the yields of ornamental plants, certain growth factors are released from porous, spherical, ceramic pellets embedded in the soil near the roots. At the surface of the pellet ($r = R$), the growth factor concentration in the soil is c_o. Far from the surface, the growth factor concentration drops to zero. Develop an expression for the steady state release rate (moles s^{-1}) of the growth factor from the pellet.

This is a case of outward diffusion from a sphere, equally in all directions. It may be easiest to approach spherical geometry using spherical coordinates.

Let us consider the 'sphere of influence' of the growth factor as our system (the roots where the growth factor is consumed are not part of the system), and use the mass concentration principle (equation of continuity). We can directly use equation C2 in Table 2.3.2-1, at steady state

$$\cancelto{0}{\frac{\partial c_A}{\partial t}} + \left(\cancelto{0\ (v_r = 0)}{v_r \frac{\partial c_A}{\partial r}} + \cancelto{0\ (v_\theta = 0)}{v_\theta \frac{1}{r}\frac{\partial c_A}{\partial \theta}} + \cancelto{0\ (v_\phi = 0)}{v_\phi \frac{1}{r\sin\theta}\frac{\partial c_A}{\partial \phi}} \right)$$

$$= D_{AB}\left(\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial c_A}{\partial r}\right) + \cancelto{0\ (c_A \neq f(\theta))}{\frac{1}{r^2\sin\theta}\frac{\partial}{\partial \theta}\left(\sin\theta\frac{\partial c_A}{\partial \theta}\right)} + \cancelto{0\ (c_A \neq f(\phi))}{\frac{1}{r^2\sin^2\theta}\frac{\partial^2 c_A}{\partial \phi^2}} \right) + \cancelto{0\ \text{(no reaction)}}{R_A}$$

Hence

$$D_{AB}\left[\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial c_A}{\partial r}\right)\right]=0$$

Since r is the only independent variable here, we can replace the partial derivatives with total derivatives. Thus

$$D_{AB}\left[\frac{1}{r^2}\frac{d}{dr}\left(r^2\frac{dc_A}{dr}\right)\right]=0 \tag{2.4.3-1}$$

If we solve the above equation, we get

$$c_A = A - \frac{B}{r} \tag{2.4.3-2}$$

The boundary conditions (BCs) are

$$\text{At } r = R,\quad c_A = c_o \tag{2.4.3-3}$$

$$\text{At } r = \infty,\quad c_A = 0 \tag{2.4.3-4}$$

Substituting the above BCs in Eq. 2.4.3-2, we get

$$c_o = A - \frac{B}{R} \text{ and } A = 0$$

Thus

$$B = -R\, c_o$$

Therefore

$$c_A = \frac{c_o R}{r} \tag{2.4.3-5}$$

The flux $$\vec{J}_A^* = -D_{AB}\left.\frac{\partial c_A}{\partial r}\right|_{r=R} = D_{AB}\left.\frac{c_o R}{r^2}\right|_{r=R}$$

Thus

$$\vec{J}_A^* = \frac{D_{AB}c_o}{R} \tag{2.4.3-6}$$

$$\begin{aligned}\text{Release rate} &= \text{Flux} \times \text{Area}\\ &= \frac{D_{AB}c_o}{R}\times 4\pi R^2\\ &= 4\pi D_{AB}c_o R\end{aligned} \tag{2.4.3-7}$$

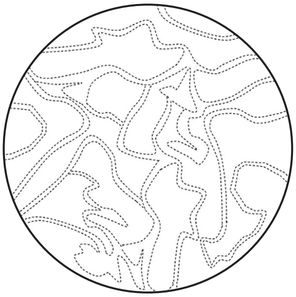


Fig. 2.4.3-1 The porous pellet

2.4.3.1 Enzyme Immobilised on a Porous Spherical Matter

Let us consider an enzyme reaction in which the enzyme is immobilised on a porous spherical pellet (Fig. 2.4.3-1). The pores could have a high surface area, say 250 m^2g^{-1}. The pellet itself is placed in a fluid environment. Since the enzyme is immobilised inside the pores of the pellet, the transfer of substrate to the site of the immobilised enzyme through the pores, and the transport of product out of the pores are expected to play a major role in determining the process kinetics. Thus, rather than considering the transport to and from the surface of the pellet, the transport inside the pores needs to be considered.

Since it is spherical pellet, let us use spherical coordinates. The relevant continuity equation (from Table 2.3.2-1, Eq. C2) applied over the spherical pellet as the system, after cancellation of the inapplicable terms, replacement of the partial derivative with an ordinary derivative because there is only one independent variable x, expansion of the only remaining term into a second order derivative and a first order derivative through chain rule for differentiation, and with Michaelis-Menten kinetics for the reaction rate, becomes

$$-D_{\text{eff}}\left[\frac{d^2s}{dr^2}+\frac{2}{r}\frac{ds}{dr}\right]=\frac{v'_{\max}s}{K'_m+s} \qquad (2.4.3.1\text{-}1)$$

Boundary conditions:

At
$$r=0, \frac{ds}{dr}=0 \qquad (2.4.3.1\text{-}2)$$

$$r = R,\ S = S_o \qquad (2.4.3.1\text{-}3)$$

The first boundary condition (Eq. 2.4.3.1-2) arises from the need for symmetry, i.e. there cannot be a discontinuity in the substrate concentration at the centre, irrespective of the direction (radius) of approach. In other words, the substrate concentration at the centre must be the same value irrespective of the direction (radius) followed to approach it. The only way that can happen is if the derivative of the substrate concentration at the centre is zero.

When certain physical quantities are combined suitably, the resulting quantity or 'number' does not possess any dimensions. There are many advantages in using non-dimensional numbers, or in expressing relations in terms of non-dimensional numbers. Such relations may become a lot more general in applicability – they will not be restricted to a particular set of values of the relevant physical variables. We will see more about non-dimensional numbers in Chapter 3.

Let us define the needed non-dimensional variables as

$$x = \frac{s}{s_o} \tag{2.4.3.1-4}$$

$$y = \frac{r}{R} \tag{2.4.3.1-5}$$

Thus

$$\frac{ds}{dr} = \frac{ds}{dx} . \frac{dx}{dy} . \frac{dy}{dr} = s_o \frac{dx}{dy} . \frac{1}{R} = \frac{s_o}{R} \frac{dx}{dy}$$

$$\frac{d^2 s}{dr^2} = \frac{d}{dr}\left(\frac{ds}{dr}\right) = \frac{d}{dy}\left(\frac{ds}{dr}\right)\frac{dy}{dr} = \frac{d}{dy}\left(\frac{s_o}{R}\frac{dx}{dy}\right)\frac{1}{R} = \frac{s_o}{R^2}\frac{d^2 x}{dy^2}$$

Thus, the differential equation becomes

$$-D_{\text{eff}}\left[\frac{s_o}{R^2}\frac{d^2 x}{dy^2} + \frac{2}{(yR)}\frac{s_o}{R}\frac{dx}{dy}\right] = \frac{v'_{\max} s_o x}{K'_m + s_o x} \tag{2.4.3.1-6}$$

Dividing throughout by $\frac{s_o D_{\text{eff}}}{R^2}$, we get

$$\frac{d^2 x}{dy^2} + \frac{2}{y}\frac{dx}{dy} = -\frac{v'_{\max} x R^2}{D_{\text{eff}}(K'_m + s_o x)}$$

or

$$\frac{d^2 x}{dy^2} + \frac{2}{y}\frac{dx}{dy} = -\frac{v'_{\max}}{D_{\text{eff}} K'_m} R^2 \left[\frac{x}{1 + \frac{s_o}{K'_m} x}\right] \tag{2.4.3.1-7}$$

Similar to non-dimensional quantities mentioned earlier in this section, one can think of non-dimensional parameters, which are useful for analysis, as will become apparent later. Let us define some non-dimensional parameters, as follows:

$$M_T = \frac{R^3 \left(\frac{v'_{\max}}{K'_m} \right) s_o}{R\, D_{\text{eff}}\, s_o} = \frac{\text{'}a\text{' reaction rate}}{\text{'}a\text{' diffusion rate}} = \text{Thiele modulus} \qquad (2.4.3.1\text{-}8)$$

$$\beta = \frac{s_o}{K'_m} \qquad (2.4.3.1\text{-}9)$$

When $s_o << K'_m$, the reaction rate is of first order. Thus, $\beta = \frac{s_o}{K'_m}$ accounts for deviation from first order kinetics. For larger values of β, the reaction is of zero order, and for smaller values of β, the reaction is of first order.

Thus, Eq. 2.4.3.1-7 can be written as

$$\frac{d^2x}{dy^2} + \frac{2}{y}\frac{dx}{dy} = -9\, M_T^2 \frac{x}{1+\beta x} \qquad (2.4.3.1\text{-}10)$$

Boundary conditions:

$$\text{At } y = 1,\ x = 1 \qquad (2.4.3.1\text{-}11)$$

$$\text{At } y = 0,\ \frac{dx}{dy} = 0 \qquad (2.4.3.1\text{-}12)$$

Solving the differential equation, we can get x vs y (or) s vs r.

We are usually more interested in determining how much the reaction is hindered due to immobilisation. To find this out, let us define an effectiveness factor that gives us a measure of the hindrance, and evaluate the same.

An effectiveness factor can be defined as

$$\xi_g = \frac{\text{Actual reaction rate}}{\text{Reaction rate in the absence of mass transfer resistance}}$$

Actual rate v_{act}: At steady state, there should be no accumulation of substrate or product at the surface. Thus, whatever substrate enters, needs to be consumed in the pellet for steady state to be valid.

$$\text{Rate of entry} = -D_{\text{eff}} \left.\frac{ds}{dr}\right|_{r=R} (-1) A_p$$

In the above equation, (– 1) is used since the outward radial direction is taken as positive (s entry is in the negative direction) and A_p is the surface area of the particle.

$$v_{\text{act}} = \frac{D_{\text{eff}}\, s_o}{R} \left.\frac{dx}{dy}\right|_{y=1} A_p$$

On a volumetric basis

$$v_{\text{act}} = D_{\text{eff}} \frac{s_o}{R} \left.\frac{dx}{dy}\right|_{y=1} \frac{A_p}{V_p} = \frac{D_{\text{eff}}\, s_o}{R} \frac{4\pi R^2}{\frac{4}{3}\pi R^3} \left.\frac{dx}{dy}\right|_{y=1}$$

$$v_{\text{act}} = 3\, D_{\text{eff}} \frac{s_o}{R^2} \left.\frac{dx}{dy}\right|_{y=1} \tag{2.4.3.1-13}$$

The reaction rate in the absence of the mass transfer resistance is the reaction rate if the concentration of the substrate is s_o. Since there is no hindrance (resistance) to the mass transport, the substrate concentration in this hypothetical situation would be the same as that at the surface of the spherical pellet.

$$\text{Reaction rate in the absence of mass transfer resistance} = \frac{v'_{\max} s_o}{K'_m + s_o} \tag{2.4.3.1-14}$$

Thus, from the previous two equations

$$\xi_g = \frac{3\, D_{\text{eff}} \dfrac{s_o}{R^2} \left.\dfrac{dx}{dy}\right|_{y=1}}{\dfrac{v'_{\max} s_o}{K'_m + s_o}}$$

$$= \frac{\left.\dfrac{dx}{dy}\right|_{y=1}}{\dfrac{R^2}{3\, D_{\text{eff}}} \dfrac{v'_{\max}}{K'_m \left(1 + \dfrac{s_o}{K'_m}\right)}}$$

$$= \frac{\left.\dfrac{dx}{dy}\right|_{y=1}}{3M_T^2 \left(\dfrac{1}{1+\beta}\right)} \tag{2.4.3.1-15}$$

2.5 Unsteady State Diffusion

In this section, unlike in the previous section, we will consider the situation when the concentration of the diffusing molecule changes with time. An example is the sorption of a surface modifying agent (SMA) on to the surface of a material. SMAs are used to promote/dissuade cellular growth on a surface of interest – it could be the hull of a ship or a container handling cell solutions. The surface is sometimes exposed to the SMA containing solution for a certain period to effect the modification.

Example 2.5-1

Let us take the case of a thin surface sorbing SMA from a solution with SMA concentration, c_o. The thin surface is placed on the bottom of the vessel containing the SMA solution. Let us consider the case where the amount of SMA sorbed is a very small fraction of the total SMA amount present in solution. In such cases, the SMA concentration far from the surface does not appreciably change (why?).

Our interest is to find the SMA concentration in solution as a function of time. It is convenient to consider rectangular coordinates here.

Taking the solution as our system, the continuity equation for SMA written on our system is Eq. A2 of Table 2.3.2-1

$$\frac{\partial c_A}{\partial t}+\left(\overset{=0\ (v_x=0)}{\cancel{v_x\frac{\partial c_A}{\partial x}}}+\overset{=0\ (v_y=0)}{\cancel{v_y\frac{\partial c_A}{\partial y}}}+\overset{=0\ (v_z=0)}{\cancel{v_z\frac{\partial c_A}{\partial z}}}\right)-D_{AB}\left(\overset{=0\ (c_A\neq f(x))}{\cancel{\frac{\partial^2 c_A}{\partial x^2}}}+\overset{=0\ (c_A\neq f(y))}{\cancel{\frac{\partial^2 c_A}{\partial y^2}}}+\frac{\partial^2 c_A}{\partial z^2}\right)=\overset{=0\ (\text{no } rxn)}{\cancel{R_A}}$$

Thus, the equation reduces to

$$\frac{\partial c_A}{\partial t}=D_{AB}\frac{\partial^2 c_A}{\partial z^2} \tag{2.5-1}$$

The initial and boundary conditions are

$$t = 0;\ z \geq 0;\ c_A = c_o \tag{2.5-2}$$

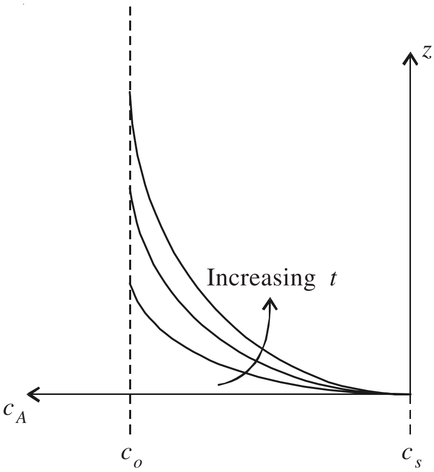
$$t \geq 0;\ z = 0;\ c_A = c_s \tag{2.5-3}$$

$$t \geq 0;\ z \rightarrow \infty;\ c_A = c_o \tag{2.5-4}$$

If we solve Eq. 2.5-1 with the above initial and boundary conditions, we can get SMA concentration profiles in the solution above the surface at various times, as shown in Fig. 2.5-1. This particular partial differential equation (PDE) can be solved by converting it into an ODE. To do that, and also to make the solution independent of the actual dimensions of each system, let us define the following dimensionless variables:

$$\theta=\frac{c_A-c_o}{c_s-c_o} \tag{2.5-5}$$

Fig. 2.5-1 The SMA concentration profiles in the liquid at various times



and

$$\eta = \frac{z}{\sqrt{4\,D_{AB}t}} \tag{2.5-6}$$

Note that we have constructed $\theta = f(\eta)$ and $\eta = f(z, t)$. While using the chain rule, $\frac{\partial\theta}{\partial\eta}$ can be replaced by $\frac{d\theta}{d\eta}$ without any loss in accuracy. The variable, η, has been constructed to allow the possibility of conversion of the partial differential equation (PDE) to an ordinary differential equation (ODE) by combining both the independent terms z and t.

Thus, using the chain rule, from Eq. 2.5-5, we get

$$\frac{\partial c_A}{\partial t} = (c_s - c_o)\frac{d\theta}{d\eta}\cdot\frac{\partial\eta}{\partial t} \tag{a}$$

Now the derivative of η with respect to t yields

$$\frac{\partial\eta}{\partial t} = \frac{\partial}{\partial t}\left(\frac{z}{\sqrt{4D_{AB}t}}\right) = \frac{-z}{2t\sqrt{4D_{AB}t}} = \frac{-\eta}{2t} \tag{b}$$

Substituting Eq. (b) in Eq. (a) we get

$$\frac{\partial c_A}{\partial t} = -(c_s - c_o)\frac{d\theta}{d\eta}\cdot\frac{\eta}{2t} \tag{c}$$

Similarly, the spatial derivatives are transformed into

$$\frac{\partial c_A}{\partial z} = (c_s - c_o)\frac{d\theta}{d\eta}\cdot\frac{\partial\eta}{\partial z} \tag{d}$$

$$\frac{\partial^2 c_A}{\partial z^2} = (c_s - c_o)\frac{\partial}{\partial z}\left[\frac{d\theta}{d\eta}\cdot\frac{\partial\eta}{\partial z}\right] \tag{e}$$

Now, since

$$\frac{\partial\eta}{\partial z} = \frac{1}{\sqrt{4D_{AB}t}}$$

is independent of *z*, we can write Eq. (e) as

$$\frac{\partial^2 c_A}{\partial z^2} = \frac{(c_s - c_o)}{\sqrt{4D_{AB}t}}\frac{\partial}{\partial z}\left(\frac{d\theta}{d\eta}\right) = \frac{(c_s - c_o)}{\sqrt{4D_{AB}t}}\frac{d}{d\eta}\left(\frac{\partial\theta}{\partial z}\right) \tag{f}$$

Applying the chain rule, we get

$$\frac{\partial\theta}{\partial z} = \frac{d\theta}{d\eta}\cdot\frac{\partial\eta}{\partial z} = \frac{1}{\sqrt{4D_{AB}t}}\frac{d\theta}{d\eta} \tag{g}$$

Substituting Eq. (g) into Eq. (f) we get

$$\frac{\partial^2 c_A}{\partial z^2} = \frac{(c_s - c_o)}{4D_{AB}t}\frac{d^2\theta}{d\eta^2} \tag{h}$$

Now by substituting Eq. (d) and Eq. (h) in Eq. 2.5-1, we get

$$\frac{-\eta(c_s - c_o)}{2t}\frac{d\theta}{d\eta} = D_{Ab}\frac{(c_s - c_o)}{4D_{AB}t}\frac{d^2\theta}{d\eta^2} \tag{i}$$

which reduces to

$$-2\eta\frac{d\theta}{d\eta} = \frac{d^2\theta}{d\eta^2} \tag{2.5-7}$$

The boundary conditions get transformed to

$$\eta = 0;\ \theta = 1 \tag{2.5-8}$$

$$\eta \to \infty;\ \theta = 0 \tag{2.5-9}$$

The variable, η, was constructed to simultaneously satisfy the initial condition (Eq. 2.5-2) and the second boundary condition (Eq. 2.5-4). Thus, we have successfully transformed a PDE into an ODE in this case. The ODE can be solved using analytical techniques. For example, let us say

$$u = \frac{d\theta}{d\eta}$$

and

$$\frac{du}{\partial\eta} = \frac{d^2\theta}{d\eta^2}$$

Therefore, Eq. 2.5-7 becomes

$$-2\eta u = \frac{du}{d\eta}$$

Recognising that the above equation can be written as

$$\frac{du}{u} = d \ln u - 2\eta\, d\eta$$

$$\ln u = -\int 2\eta\, d\eta$$

$$\ln u = -\eta^2 + A$$

Therefore

$$u = \frac{d\theta}{d\eta} = C_1 \exp(-\eta^2)$$

This cannot be integrated analytically, except by series expansion

$$e^{-\eta^2} = 1 - \frac{\eta^2}{1!} + \frac{\eta^4}{2!} - \frac{\eta^6}{3!} + \ldots$$

which, when integrated, yields

$$\int e^{-\eta^2} d\eta = \eta - \frac{\eta^3}{3\times 1!} + \frac{\eta^5}{5\times 2!} - \frac{\eta^7}{7\times 3!} + \ldots + C$$

We can get at the solution through another route; let us keep the integral signs for a few more steps. Integration yields

$$\theta = C_1 \int \exp(-\eta^2)\, d\eta + C_2 \tag{a$'$}$$

Applying the boundary conditions

$$\eta = 0;\ \theta = 1$$

$$\eta \to \infty;\ \theta = 0$$

we get

$$1 = C_1 \int \exp(-\eta^2)\, d\eta\Big|_{\eta=0} + C_2 \tag{b$'$}$$

$$0 = C_1 \int \exp(-\eta^2)\, d\eta\Big|_{\eta\to\infty} + C_2 \tag{c$'$}$$

Eliminating C_2 from the above two equations, we get

$$-1 = C_1\left\{\int \exp(-\eta^2)\,d\eta\Big|_{\eta\to\infty} - \int \exp(-\eta^2)\,d\eta\Big|_{\eta=0}\right\}$$

$$= C_1\int_0^{\infty} \exp\,(-\eta^2)\,d\eta \qquad \text{(d}'\text{)}$$

Since a series expansion provides

$$\exp(-\eta^2) = 1 - \eta^2 + \frac{\eta^4}{2!} - \frac{\eta^6}{3!} + \ldots$$

the series expansion can be substituted into the integral for evaluation. The above *definite* integral, which is useful in many situations, is called the *error function*. The values of the integral between a lower limit of 0, and various upper limits, are available in standard mathematical tables. When the expression is evaluated by expanding the series, or by using the error function values, the value $\frac{\sqrt{\pi}}{2}$ is got.

Thus, from Eq. (d′)

$$C_1 = -\frac{2}{\sqrt{\pi}}$$

Eliminating C_2 from equation (a′) and (b′) gives

$$\theta - 1 = C_1\left\{\int \exp(-\eta^2)\,d\eta\Big|_{\eta=\eta} - \int \exp(-\eta^2)\,d\eta\Big|_{\eta=0}\right\}$$

$$\theta = 1 + C_1\int_0^{\eta} \exp(-\eta^2)\,d\eta$$

We need to differentiate between η in the limit on the integral in the equation above, and the η in the integrand. The η in the integrand is a variable, which can be replaced by another variable, say *x*, to give the same meaning. Thus

$$\theta = 1 - \frac{2}{\sqrt{\pi}}\int_0^{\eta} \exp(-\eta^2)\,d\eta = 1 - \frac{2}{\sqrt{\pi}}\int_0^{\eta} \exp(-x^2)\,dx$$

or

$$\theta = 1 - \text{erf}\,(\eta)$$

$$\theta = \text{erfc}\,(\eta)$$

where erfc (η) is the complementary error function which is defined as 1 – erf (η). Replacing the non-dimensional variables with their dimensional equivalents, we get

$$\frac{c_A - c_o}{c_s - c_o} = \operatorname{erfc}\left(\frac{z}{\sqrt{4D_{AB}t}}\right) \tag{2.5-10}$$

Thus, c_A will vary as shown in Fig. 2.5-1.

The flux

$$\vec{J}_A^* = -D_{AB}\left.\frac{\partial c_A}{\partial z}\right|_{z=0} = -D_{AB}(c_s - c_o)\left.\frac{\partial \theta}{\partial z}\right|_{z=0}$$

$$= -D_{AB}(c_s - c_o)\left.\frac{d\theta}{d\eta}\frac{\partial \eta}{\partial z}\right|_{z=0}$$

$$\vec{J}_A^* = \frac{-D_{AB}(c_s - c_o)}{\sqrt{4D_{AB}t}}\left.\frac{d\theta}{d\eta}\right|_{\eta=0} \tag{2.5-11}$$

The Leibnitz rule provides the means for differentiating an integral. It says that if

$$I(t) = \int_{a_1(t)}^{a_2(t)} f(x,t)\, dx$$

then

$$\frac{dI}{dt} = \frac{d}{dt}\int_{a_1(t)}^{a_2(t)} f(x,t)\, dx$$

$$= \int_{a_1(t)}^{a_2(t)}\left(\frac{\partial}{\partial t} f(x,t)\right)dx + f(a_2(t),t)\frac{da_2}{dt} - f(a_1(t),t)\frac{da_1}{dt}$$

Thus, in this case, since

$$\theta = 1 - \frac{2}{\sqrt{\pi}}\int_0^{\eta}\exp(-x^2)\,dx$$

the derivative that is needed in Eq. 2.5-11 is

$$\frac{d\theta}{d\eta} = 0 - \frac{d}{d\eta}\left[\frac{2}{\sqrt{\pi}}\int_0^{\eta}\exp(-x^2)\,dx\right]$$

According to the Leibnitz rule

$$\frac{d\theta}{d\eta} = \frac{-2}{\sqrt{\pi}}\left[\int_0^{\eta}\frac{\partial}{\partial \eta}\exp(-x^2)\,dx + \exp(-\eta^2)\frac{d\eta}{d\eta} - \exp(-0^2)\frac{d0}{d\eta}\right]$$

Since the function inside the integral is not a function of η, the first term is zero, and the last term is zero. Thus

$$\frac{d\theta}{d\eta} = \frac{-2}{\sqrt{\pi}}\exp(-\eta^2)$$

At $\eta = 0$

$$\left.\frac{d\theta}{d\eta}\right|_{\eta=0} = \left[-\frac{2\exp(-\eta^2)}{\sqrt{\pi}}\right]_{\eta=0} = -\frac{2}{\sqrt{\pi}}$$

Therefore, the flux

$$\vec{J}_A^* = \sqrt{\frac{D_{AB}}{\pi t}}(c_s - c_o) \tag{2.5-12}$$

2.6 Pseudo Steady State Approximation (PSSA) for Unsteady State Diffusion

To understand pseudo steady state approximation, let us consider the processes involved in manufacturing a car. We will focus on three of the processes as shown below

Process	Characteristic rates
Making the bolts that are used in the engine	Say, 1 bolt per 5 s
Making the engine	Say, 1 engine per 1 h
Making the whole car	Say, 1 car per 10 h

If our interest is in engine-making, the process of bolt-making is fast enough to be considered at pseudo steady state, i.e. the changes in the rate of bolt-making (unsteady aspects) will not much affect the rate of engine-making. Also, the rate of whole-car-making is so slow, that it is not relevant to the rate of engine-making. Thus, for the interest at hand, i.e. engine-making, the process of whole-car-making can be taken as ‘frozen’.

Now, let us shift our attention to cellular processes.

Process	Characteristic rates
Enzyme action	One in every 10^{-3} s
Cell growth/division	One in every 10^2 s
Natural mutation	One in every 10^8 s

If we are interested in cell growth/division, enzyme action can be taken to be at pseudo steady state, and natural mutation can be considered ‘frozen’.

Now, let us consider a thin membrane through which diffusion of a species occurs. Take the membrane as the system of interest. If the diffusion through the membrane is fast enough compared to the changes in the concentration of the species at the membrane surfaces (in the bulk solutions), then the diffusion through the membrane can be assumed to take place under steady state conditions when the interest is in the concentrations at the membrane surfaces (in the bulk solutions) i.e. $\frac{\partial c_m}{\partial t}$ can be approximated to be zero. This is called the pseudo steady state approximation (PSSA).

Example 2.6-1

As seen in Section 2.5, coatings can improve cell adherence to surfaces. Let us consider a coated porous surface on which cells are grown. Let us also consider the case in which a growth factor in the medium needs to pass the porous surface and the coating to reach the cells and ensure good growth.

The permeability of the growth factor through the coating needs to be determined. Permeability can be measured using a cylindrical vessel separated into two chambers, *A* and *B*, by the material whose permeability is being measured. Since the coating on the porous surface is too thin to have the necessary mechanical properties to act as the above-mentioned separator between the two chambers, another technique is used to find the needed permeability.

The permeability of a membrane with suitable mechanical properties is first measured. Then, the permeability of the membrane with the 'coating' is measured. The membrane used in the experiment is circular with an area of 1.33 cm^2 and the volume of each chamber (*A* or *B*) is 2 cm^3. The initial concentration of the growth factor in chamber *A* at the start of the experiment is 10 mg l^{-1}, and in chamber *B*, 0. The growth factor concentration in chamber *B* at different times from the start of the experiment are given in mg l^{-1} in the following format below: time in minutes (concentration with membrane, concentration with coated membrane)

0 (0, 0); 20 (0.4, 0.01); 40 (0.7, 0.02); 80 (1.3, 0.035)

We need to determine the growth factor permeability of the coating under PSSA, since the rate at which the concentration of the growth factor in *B* changes is usually much slower than the rate at which the growth factor moves through the membrane.

The solution strategy is to consider the membrane and the coating to be 'membranes in series'. Thus, their resistances, or the inverse of their conductances (permeabilities) are additive. Permeability is equal to *DK/L*, where *D* is the diffusivity, *K* is the partition coefficient and *L* is the membrane thickness. The permeabilities need to be found from the given data of concentrations at various times.

Let us first consider the membrane as our system. Application of the equation of continuity (Eq. A2 from Table 2.3.2-1) for A on this system of interest (the membrane) yields

$$\overset{=0\ (PSS)}{\cancel{\frac{\partial c_A}{\partial t}}} + \left(v_x \overset{=0\ (v_x=0)}{\cancel{\frac{\partial c_A}{\partial x}}} + v_y \overset{=0\ (v_y=0)}{\cancel{\frac{\partial c_A}{\partial y}}} + v_z \overset{=0\ (v_z=0)}{\cancel{\frac{\partial c_A}{\partial z}}} \right) - D_{AB}\left(\frac{\partial^2 c_A}{\partial x^2} + \overset{=0\ (c_A \neq f(y))}{\cancel{\frac{\partial^2 c_A}{\partial y^2}}} + \overset{=0\ (c_A \neq f(z))}{\cancel{\frac{\partial^2 c_A}{\partial z^2}}} \right) = \overset{=0\ (\text{no } rxn)}{\cancel{R_A}}$$

Thus, we get

$$D_m \frac{\partial^2 c_m}{\partial x^2} = 0 \tag{2.6-1}$$

where the subscript m implies the membrane, c_m is the concentration of A in the membrane and D_m is the diffusivity of A in the membrane.

We had earlier seen (Eq. 2.4.1-7) the solution of the above DE to be

$$c_m = Kc_A - K(c_A - c_B)\frac{x}{L} \tag{2.6-2}$$

and the flux

$$\vec{N}_A = \vec{J}_A^{*} = -D_m \frac{dc_m}{dx} = \frac{D_m K}{L}(c_A - c_B) \tag{2.6-3}$$

Now, let us call our species A as i (to avoid difficulties with compartment A) and apply the mass balance of the species i on the compartment A; we get

$$\frac{dA_i}{dt} = \overset{=0}{\cancel{\dot{I}_i}} - \dot{O}_i + \overset{=0}{\cancel{\dot{G}_i}} - \overset{=0}{\cancel{\dot{C}_i}}$$

The output rate of species i needs to be equal to the transfer rate of the species, i through the membrane.

Since the flux of i through the membrane is $\frac{D_{i,m}K}{L}(c_A - c_B)$, and the rate = area × flux

$$\text{Rate} = \frac{A_m D_{i,m} K}{L}(c_A - c_B) \tag{2.6-4}$$

Thus, the mass balance of i becomes

$$\frac{dA_i}{dt} = \frac{d(V_A c_A)}{dt} = \frac{-A_m D_{i,m} K}{L}(c_A - c_B)$$

Since V_A is constant

$$V_A \frac{dc_A}{dt} = \frac{-A_m D_{i,m} K}{L}(c_A - c_B) \tag{2.6-5}$$

A mass balance of i on the entire vessel consisting of the compartment A and B, and the membrane, yields

$$\frac{dA_i}{dt} = \cancelto{=0}{I_i} - \cancelto{=0}{O_i} + \cancelto{=0}{G_i} - \cancelto{=0}{C_i}$$

i.e.

$$\frac{dA}{dt} = 0$$

When each compartment and the membrane are explicitly expressed, the above equation becomes

$$\frac{d(V_A c_A)}{dt} + \frac{d(V_B c_B)}{dt} + \frac{d\left(V_m \dfrac{c_m}{K}\right)}{dt} = 0$$

The partition coefficient K is used to represent all concentrations in consistent units. Note that the units of c_A or c_B = moles of i/volume of solution in chamber A or B, and that the partition coefficient converts the concentration of i in the membrane into the equivalent solution concentration.

Since the volumes are constant

$$V_A \frac{d(c_A)}{dt} + V_B \frac{d(c_B)}{dt} + \frac{V_m}{K}\frac{dc_m}{dt} = 0 \tag{2.6-6}$$

By pseudo steady state approximation, $\frac{dc_m}{dt} = 0$. Also, we know that V_A = V_B. Thus

$$\frac{dc_A}{dt} = \frac{-dc_B}{dt} \tag{2.6-7}$$

Using the initial conditions (at t = 0)

$$c_A = c_o \tag{2.6-8}$$

$$c_B = 0 \tag{2.6-9}$$

If we integrate Eq. 2.6-7, we get

$$c_A - c_o = -c_B \tag{2.6-10}$$

Substituting Eq. 2.6-8 in Eq. 2.6-5, we get

$$A_m D_{i,m} K \frac{(2c_A - c_o)}{L} = -V_A \frac{dC_A}{dt} \tag{2.6-11}$$

Integrating Eq. 2.6-11 with the initial conditions $c_A = c_o$, we get

$$\frac{-2A_m D_{i,m} K}{V_A L} t = \ln\left(\frac{2c_A - c_o}{c_o}\right) \tag{2.6-12}$$

A plot of ln $\left(\frac{2c_A - c_o}{c_o}\right)$ vs. t provides a line of slope $\frac{-2A_m D_{i,m} K}{V_A L}$.

Now, recall that the permeability P is defined as (Section 2.4.1) $\frac{DK}{L}$. Thus

$$P_m = \frac{D_m K}{L_m} \tag{2.6-13}$$

and let us say that P_{cl} is permeability of the coated layer. Since the membrane and coated layer act in series for the transport of the growth factor, when both are present, their resistances (inverse permeability values) are additive

$$\frac{1}{P_{\text{Total}}} = \frac{1}{P_m} + \frac{1}{P_{cl}} \tag{2.6-14}$$

Thus, if the data is used to plot ln $\left(\frac{2c_A}{c_o} - 1\right)$ vs time, use of the first data points in the brackets given in the problem statement (with the membrane alone) gives $\frac{-2A_m P_m}{V_A}$ as the slope and the second data points in the brackets (membrane + coating) gives $\frac{-2A_T P_T}{V_A}$. Equation 2.6-14 can then be used to determine the permeability of the coating.

The value: $P_m = 4.8 \times 10^{-5}$ cm s^{-1}, $P_T = 1.1 \times 10^{-6}$ cm s^{-1}. Therefore $P_{cl} = 1.08 \times 10^{-6}$ cm s^{-1}. (Almost the entire resistance for the growth factor flux in the evaluation system is provided by the coating).

Exercises

1. Succinctly, differentiate between the following:
   (a) Conservation equation and constitutive equation
   (b) Driving force and flux
   (c) Mass average velocity and molar average velocity
   (d) Steady state and unsteady state
   (e) Steady state and pseudo steady state
   (f) Fick's first and second laws

2. For a binary system of A and B, show that the following relationships hold:

   (a) $\vec{v} = \frac{1}{\rho}(\rho_A \vec{v}_A + \rho_B \vec{v}_B) = w_A \vec{v}_A + w_A \vec{v}_B$

   (b) $\vec{v}^* = \frac{1}{c}(c_A \vec{v}_A + c_B \vec{v}_B) = x_A \vec{v}_A + x_B \vec{v}_B$

   (c) $\vec{v} - \vec{v}^* = w_A(\vec{v}_A - \vec{v}^*) + w_B(\vec{v}_B - \vec{v}^*)$

   (d) $\vec{v}^* - \vec{v} = x_A(\vec{v}_A - \vec{v}) + x_B(\vec{v}_B - \vec{v})$

   (e) $\vec{n}_A + \vec{n}_B = \rho\vec{v}$

   (f) $\vec{N}_A + \vec{N}_B = c\vec{v}^*$

   (g) $\vec{j}_A + \vec{j}_B = 0$

   (h) $\vec{J}_A^* - \vec{J}_B^* = 0$

3. A test tube containing pure ethanol was accidentally left open in a room at 32 °C. The length of the test tube was 15 cm, and the length of the ethanol column at the bottom was 2 cm. Diffusivity of ethanol in air is 0.135 cm^2 s^{-1}. Derive an expression for the partial pressure of ethanol as a function of the height in the test tube, under steady state conditions. Assume that air is insoluble in ethanol, and that the vapour pressure of ethanol at 32 °C is 7853 Pa.

4. A small amount of medicated gel is applied to a reasonably large area of the skin – thus, we can consider the transfer of the active ingredient into the skin as a one dimensional process in Cartesian coordinates. The skin is 2 mm thick. If the effective concentration of the active ingredient at the surface of the skin for the time of interest can be assumed to remain constant at C_s – the constancy can be assumed if the amount transported into the skin is much less than the amount originally in the gel – and the concentration at a depth of 1.75 m is C_a, find the concentration profile of the active ingredient in the skin. The diffusivity of the active ingredient in the skin was found to be D_A.

5. The Kirby Bauer test is a test that uses antibiotic impregnated wafers to test the susceptibility of bacteria to that particular antibiotic. The antibiotic disc is placed in the middle of an agar plate that has been streaked with the bacterial suspension. Upon incubation, a zone of clearance (no growth) is observed if the bacteria are susceptible to the antibiotic. The minimum inhibitory concentration (MIC) is the lowest concentration of an antibiotic that will inhibit the visible growth of a microorganism.

   In one of the Kirby Bauer test, 2 mm discs with an equivalent (in the agar) ampicillin concentration of 10 μg ml^{-1} was used on a strain. The MIC is 2 μg ml^{-1}. The diameter of the zone of clearance on the agar plate was 25 mm. Assuming that the amount of ampicillin in the agar medium is much less than that originally present on the disc, find the concentration profile of ampicillin in the zone of clearance.

6. An agar nutrient medium taken in a test tube is inoculated with bacteria which has no kanamycin resistance. Assume uniform inoculation throughout the volume of the agar. A disc containing uniformly distributed kanamycin is placed at the open end of the agar medium, in the test tube. The growth of the bacteria is observed after 24 h. If the minimum inhibitory concentration of the bacteria is known to be c_o M, find the length upto which bacterial growth will take place. Assume that the total amount of kanamycin in the medium is much less than the amount originally present on the disc.

7. A disc shaped piece of wood is floating down the river (transport of wood by river flow is common). The piece has a radius of 1 m, a thickness of 0.1 m, and weighs 125 kg when it is dry. Water diffuses through the wood, and let us say that a steady state has been achieved. Assuming that no water is present on the exposed (upper) surface of the wood, find the effective density of that wood piece. Neglect humidity and take the diffusivity of water in wood to be 5×10^{-6} cm^2 s^{-1}.

8. Tapeworms are flatworms that can infect human intestines. They do not have a separate respiratory system. They take in oxygen directly from their environment through an envelope consisting of an ectoderm and an endoderm. If the diffusivity of oxygen through the ectoderm is D_1, and through the endoderm is D_2, the oxygen concentration in the environment is C_o, and that needed inside the worm is C_i, find the steady state oxygen concentration profile in the tapeworm envelope.

9. Aluminium is toxic to plants, and its presence in the soil affects the growth of its roots. Plants have adapted to this by secreting citrate, which chelate aluminium, and prevent its entry into the roots. Calculate the steady state molar flux of citrate through the hemispherical root tip. Take the radius of the outer surface of the root tip to be R_{outer}, and that of the inner surface to be R_{inner}. At steady state, the aluminium concentration on the membrane at the inner root tip surface is 200 μM, and that at the outer root tip surface can be approximated to be zero.

10. An artery has inner and outer radii, r_1 and r_2, respectively. The diffusivity of oxygen varies as follows across the cross-section of the arterial wall

$$D(r) = \frac{D_0}{r}$$

The artery needs to be replaced by an artificial one, and the artificial artery has a membrane diffusivity of D_0 uniformly across the cross-section of its wall. What is the thickness of the artificial artery if it needs to function similar to the natural one in terms of oxygen delivery transport across its wall?

11. The bird embryo inside the egg takes its oxygen from the air. The process by which oxygen reaches the embryo is diffusion across the relatively porous shell, and the not so porous membrane just beneath the shell. Assuming the membrane thickness to be 100 μ, the partition coefficient for oxygen in this system to be unity, make a rough estimate of the flux of oxygen across the membrane at a steady state concentration of oxygen inside the egg (due to consumption by the embryo) of 60 % of the saturated value in the fluid surrounding the embryo inside the egg. For the purposes of this estimate, assume that the fluid properties are the same as that of water.

12. To improve yields of ornamental plants, certain growth factors are released from porous, spherical, ceramic pellets embedded in the soil near the roots. At the surface of the pellet ($r = R$), the growth factor concentration in the soil is C_0. Far from the surface, the growth factor concentration drops to zero. The growth factor is thus delivered by pure diffusion to the roots. Nevertheless, the growth factor degrades while in the soil before it reaches the roots, in a first order fashion with a degradation constant, k_d. Set up the governing equation to describe the transport of the growth factor in the soil, along with the appropriate boundary conditions.

13. In a certain process, mammalian cells grow inside porous microcarrier beads of radius, R. A particular substrate, A, is crucial for the desired growth of the cells under these conditions, and hence there is an interest in determining the concentration distribution of A inside the bead. The effective diffusivity of A inside the pores of the bead is D_A. The 'growth reaction' can be considered as first order with respect to A, with an appropriate first order rate constant, k. If the concentration on the surface of the bead is C_{As}, set up the differential equation and the appropriate boundary conditions, which will be needed to obtain an expression for the concentration distribution of A inside the bead.

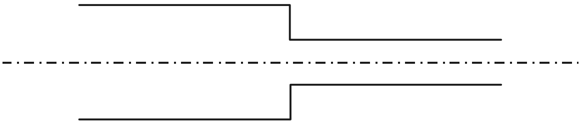
14. When the liquid phase oxygen supply strategy (LPOS) was used to cultivate *A. niger* (mould), under certain conditions, a pellet morphology was observed. The hydrogen peroxide added in the extracellular medium, diffuses into the porous pellet, and breaks down inside the pellet to release oxygen. Set up the equation and the boundary conditions to obtain the oxygen profile in the pellet under the above conditions. Assume that the needed parameters are known.

15. When bacterial cells are made competent and placed in a medium with plasmid DNA, the DNA diffuses through the plasma membrane. Due to competence, pores are formed and the DNA rushes through these pores.

Derive an expression to find the permeability of DNA through the membrane when the flow rate through the pores is equal to the diffusive flux through the membrane. Assume that the cells are cylindrical bacterial cells with pores present only along the curved surface of the cylinder.

16. Cyclosporin is an immunosuppressant drug. It acts by binding to the cytosolic protein, cyclophilin, in the *T*-lymphocytes. At steady state, cyclosporin concentration in the blood is C_o, and its concentration in the cytosol of the lymphocyte is C_i. Assuming lymphocytes to be spherical in shape with external radius, r_o, and internal radius, r_i, derive an expression for the molar flux of cyclosporin into the lymphocyte. The diffusivity of cyclosporin across the lymphocyte membrane is D; its partition coefficient in the lymphocyte membrane is K.

17. Can the continuity equations in the form given in Table 2.3.2-1 be applied when there is a change in cross-sectional area in the direction of transport, such as in the case of a sudden contraction?



18. Two rivers, say Adyar and Cooum, flowing in the same direction toward the sea, are separated by a distance, L, in a certain Chennai region. In that region, the concentration of nickel in the Adyar river is C_A and that in the Cooum river is C_C; assume, $C_C > C_A$. A cylindrical connection between the two rivers is made so that the connector length is L, and its diameter is D. Another connection, in the shape of the frustum of a cone is also made between the two rivers. The length of the second connector is also L, and its diameter, d, varies linearly with distance along its axis, x, as follows:

$$d = d_C(1 + kx)$$

d_C = the diameter at the Cooum end, and $k = (2L)^{-1}$. Assuming that the waters in the connectors are still (no convection) and that no relevant chemical reaction takes place, derive an expression for the steady state mole flux of nickel as a function of x, in (a) the cylindrical connector, and (b) the frustum of the cone connector. The diffusion coefficient of nickel in the river water is D_{Ni}.

19. Somewhere upstream of the Adyar river compared to the position in the previous exercise, the government decided to cultivate prawns using the river water, in a cuboidal pond just next to the river. The size of the prawn cultivation pond was 75 × 50 × 3 m^3, and the connector that brought in river water for the cultivation into the pond was again cuboidal of size 5 × 5 × 2 m^3. A nickel concentration of say, 5 ppm is toxic to prawns. Assuming that there was no

nickel present initially in the cultivation pond (and the river), if the concentration in the river rises suddenly to a steady value of 10 ppm, how long will it take for the nickel in the prawn cultivation pond to reach toxic levels. Also assume that the waters in the prawn cultivation pond and the cuboidal connector are still.

20. A normal person gets a small cut and starts bleeding. The clotting process to stop the blood loss through the cut begins immediately. The clot can be looked at as a fibrous structure with a pore size that reduces with the progression of the clot formation, and the blood can be assumed to permeate through the clot while the bleeding is on. When the pore size in the clot reduces to that of the RBC radius, *a*, the bleeding can be expected to end. If the reduction in pore radius happens from an initial radius of r_0, as follows

$$r(t) = r_0(1 + \exp(-\lambda t))^{-1}$$

estimate (a) permeability as a function of time, (b) clotting time, and (c) total blood lost.

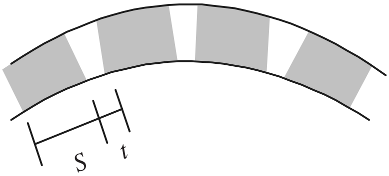
21. Facilitated diffusion is a process by which some proteins such as permeases on the membrane help in the transfer of substrate molecules across the membrane without explicit energy expenditure through ATP breakdown (passive transport). The process of facilitated diffusion can be viewed as an enzyme reaction that follows Michaelis-Menten kinetics. Derive an equation for substrate transport through facilitated diffusion. Verify the model using the following results for a substrate, *S*; take v_{max} = 0.14 mmole (mg-protein min)$^{-1}$

Time (s)	Intracellular *S* level, mole (mg-protein)$^{-1}$
150	0.12
300	0.22
450	0.28
600	0.33

22. A substrate, *S*, diffuses through a membrane, and gets converted to a product through a zero order reaction that occurs in the membrane. Derive an expression for the concentration of *S* with time in the membrane. Do you notice anything curious about the expression?

23. The root envelope tissue in plants can be visualised as consisting of layers of cylindrical sheets, one over the other. Each of those cylindrical sheets are made of membranes with pores. Thus, in cross-section, a part of each idealised sheet would appear as membranes of width *s*, separated by pores of pore diameter, *t*, as shown in the figure. Take the inner and outer radii of curvature for the two arcs of the circles to be R_b and R_c, respectively. What

is the effective diffusion coefficient for, say a nutrient, in such a structure? Also develop an expression for the concentration profile of the nutrient in the envelope.



24. The pulmonary artery carries deoxygenated blood to the lungs, and the pulmonary vein carries oxygenated blood from the lungs. The transfer of oxygen from the lungs to the blood in the vasculature, and the transfer of carbon dioxide from the vasculature to the lungs happens at the microscopic spherical ends of the gas pathway in the lungs, namely alveoli. The gases pass through the alveolar wall, basement membrane, and the vascular wall during the transfer process. Derive an expression for the flux of these gases in terms of their permeabilities through the three structures, i.e. alveolar wall, basement membrane and the vascular wall. Taking the partial pressure of oxygen in the alveoli as 100 mm Hg, and that in the vasculature as 40 mm Hg, estimate the oxygen flux. Also, taking the partial pressure of carbon dioxide in the vasculature as 45 mm Hg and that in the alveoli as 40 mm Hg, estimate the carbon dioxide flux.

25. Valinomycin is a potent toxin. It acts by destabilising the membrane potential. It binds with K^+ with a very high affinity and shields its charge. As a result, K^+ ions diffuse through the cell membrane as ‘uncharged’ species. Estimate the time taken for the intracellular K^+ concentration to reduce to half its initial level of 100 mM. The extracellular K^+ concentration can be taken to be constant at 10 mM during this process (large extracellular volume, and hence the addition of valinomycin-K^+ complex molecules from the intracellular space does not appreciably change the concentration). It can be assumed, for initial estimates, that the concentration of the complex is the same as the K^+ concentrations, in the extra- and intra-cellular spaces. The partition coefficient of the complex between the membrane and the cytoplasm is 0.8, which can be assumed to be the same on the extracellular side too. The diffusivity of the uncharged valinomycin-K^+ complex in the membrane can be taken to be 4×10^{-7} cm^2 s^{-1}. The cell can be taken to be a sphere of radius 0.5 μ, and membrane thickness, 10 nm.

Some of the above exercise problems were suggested/formulated by G. Shashank, G. Vivek Sathvik, D. Divya Vani, I. Pradeep Kumar (3), Chaitra Prabhakar, Ashritha Durvasula, Pasupuleti Sai Shalini, K.M. Sandeep, Sattu Kishore (5, 21, 22, 24), S. Kousik, Sagar Laygude, Utsav Saxena, G. Vigneshwaran, Dinesh Babu (6, 10), P. Raghavendran, P. Vivek, K. Ramasamy, M. Ashok (7, 9, 16, 25), Ayush Varma, Varun Chokshi, Dharav Solanki, T. Jaikiran (8), T. Avaneesh, Sonia Chottani, Ramaganesh, Roopteja, Moutushi Das (15, 20), Uma Maheswari, Namrata Kamat, Kiran, Kemun Khimun and Rashmi Kumari (23).

Fully Open-ended Exercise

When should a face mask that is used to protect people against poisonous gases be replaced? This problem was formulated by Aditi Jain, for her CFA exercise on a face mask designed for depleted uranium (CFA stands for choose-focus-analyse exercise; see end of Chapter 1 for a relevant reference). Aditi's report can be found as a link from www.biotech.iitm.ac.in/GK_research.

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Part II

Momentum Conservation

Chapter 3
Momentum Flux

We have seen in Chapter 1 that a fluid (either a gas or a liquid) is a substance that takes the shape of the vessel containing it. We have also seen that all real fluids have a property called viscosity associated with them.

Let us consider two parallel flat plates with a fluid (say water) in between them. Now let us consider the situation when the bottom plate is carefully moved in the x direction with a reasonably small velocity, v_x. If the velocity is small enough, we can assume that the bottom-most liquid layer adhering to the plate will also move with the same velocity as that of the plate. The shear stress due to the shear force exerted by the bottom-most layer of fluid influences the velocity of the fluid layer above it. The shear stress exerted by the layer above the bottom-most layer influences the velocity of the layer above it, and so on. The resulting steady state velocity profile of the fluid between the two plates is given in Fig. 3-1.

Stress is denoted by τ_{yx}, where yx refers to the fact that the stress (force per unit area) that arises due to a force acting in the x direction on a surface, causes an effect in the y direction. Thus, τ_{yx} is a shear stress – the direction of effect is orthogonal to the direction of motion, and, as we shall better understand later, τ_{xx} is a normal stress. The idea of the flow being in layers as shown in Fig. 3-1, and the shear stress idea subsequently conveyed are simplistic, only for didactic purposes. We will make the ideas more general when needed, later in the chapter.

It can be recalled that the shear or normal stress is force per unit area, and that force is rate of momentum change (from Newton's second law). Or

$$\begin{aligned}\tau_{yx} = \frac{\text{Force}}{\text{Area}} &= \frac{\text{MLT}^{-2}}{\text{L}^2} = \frac{[\text{M}(\text{LT}^{-1})]\,\text{T}^{-1}}{\text{L}^2}\\ &= \frac{\text{Rate of momentum change}}{\text{Area}}\\ &= \text{Momentum flux}\end{aligned}$$

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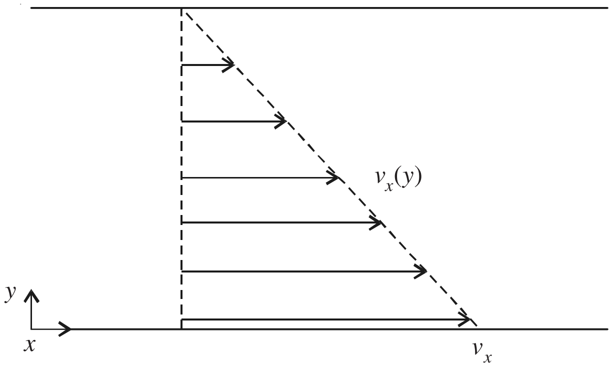


Fig. 3-1 Velocity distribution of a fluid between two parallel, closely spaced plates with the bottom plate being moved at a velocity, v_x

Note that although the direction of action is orthogonal in the example mentioned above, the change happens in the *x momentum* of the subsequent layers.

3.1 Rheology

The relationship between the shear stress, τ_{yx} and a 'shear rate', or velocity gradient $\frac{dv_x}{dy}$ was experimentally observed by Isaac Newton as

$$\tau_{yx} = -\mu \frac{dv_x}{dy} \tag{3.1-1}$$

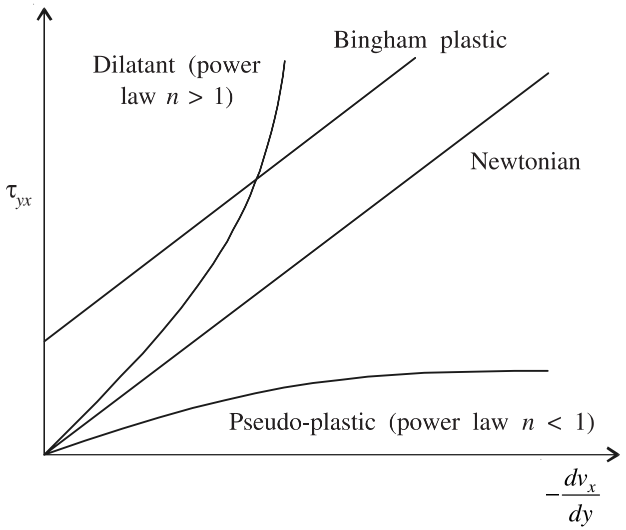
The constant of proportionality, μ, is called viscosity, and is a fundamental material property. Readers interested in acquainting themselves with the methods to estimate viscosity of gases and liquids, and to evaluate the effect of temperature and pressure on viscosity can refer to books like *Transport Phenomena* (Bird et al. 2002). The above equation is a constitutive equation, and is called the 'Newton's law of viscosity'. Recall that Fick's I law was also a constitutive equation. As generalised in Section 2.2.1, it follows the following relationship: Flux is proportional to the gradient of its primary driving force.

Dimensionally, shear stress can be written from the introductory section as

$$\left(\frac{\mathrm{MT}^{-1}}{\mathrm{L}}\right)\left(\frac{(\mathrm{LT}^{-1})}{\mathrm{L}}\right)$$

Thus, the dimensions of viscosity are $\mathrm{ML}^{-1}\mathrm{T}^{-1}$.

Fig. 3.1-1 The shear stress-shear rate behaviour of various fluid types



If we plot τ_{yx} vs $\left(\frac{dv_x}{dy}\right)$ for the above fluid (water), we get a straight line passing through the origin as shown in Fig. 3.1-1. Fluids that exhibit such behaviour are known as Newtonian fluids. As can be expected, not all fluids are Newtonian – they may exhibit different stress-shear rate behaviours. Nevertheless, a Newtonian fluid approximation is a good one for many fluids under certain conditions.

Bingham Plastic

A Bingham plastic fluid exhibits a rheology different from a Newtonian one. It does not flow until a certain minimum shear stress, τ_0, is applied i.e. the shear rate is zero until $\tau_{yx} < \tau_0$. τ_0 is called the ‘yield stress’ for the material.

It can be represented as

$$\tau_{yx} = \tau_0 - \mu \frac{dv_x}{dy} \quad \text{if } |\tau_{yx}| > \tau_0 \tag{3.1-2a}$$

$$\frac{dv_x}{dy} = 0 \quad \text{if } |\tau_{yx}| < \tau_0 \tag{3.1-2b}$$

Power Law Fluids

Newtonian fluids and Bingham plastics have viscosities that are independent of shear rate. Some fluid viscosities, though, are dependent on their shear rates. This means that the fluid will either become easier to flow, or more difficult to flow, with an increase in shear rate. Such fluids are known as power law fluids because the variation of a particular, 'apparent viscosity' with shear rate, is expressed as a power law

$$\tau_{yx} = -m\left|\frac{dv_x}{dy}\right|^{n-1}\frac{dv_x}{dy} \tag{3.1-3}$$

where the apparent viscosity, μ_{app}, is given as

$$\mu_{\text{app}} = m\left|\frac{dv_x}{dy}\right|^{n-1} \tag{3.1-4}$$

where m and n are parameters that are dependent on the fluid.

- If $n = 1$, the fluid is Newtonian and $m = \mu$ (Newtonian viscosity)
- If $n < 1$, the fluid is shear-thinning or pseudo-plastic
- If $n > 1$, the fluid is shear-thickening or dilatant

Viscoelastic Fluids

Some fluids show time-dependent behaviour – the shear stress depends on the shear rate (viscous) as well as on the strain (elastic or Hookean). A common constitutive equation to describe viscoelastic fluids is the Maxwell model

$$\tau_{yx} + \frac{\mu}{G}\frac{\partial \tau_{yx}}{\partial t} = \mu\left(-\frac{dv_x}{dy}\right) \tag{3.1-5}$$

where G is the shear elastic modulus (Nm^{-2}).

The synovial fluid that lubricates joints in the human body shows viscoelastic behaviour. It is a complex fluid consisting of proteins out of which hyaluronic acid is the most important. Mucus and vitreous fluid in the eye also show viscoelastic behaviour.

Blood

Blood is a complex biological fluid that consists of plasma, which is a mixture of liquids, proteins, with cells such as erythrocytes, leukocytes, and others suspended in it. It behaves partially as a Bingham plastic, i.e. it exhibits a yield stress, and partially as a viscoelastic fluid. Besides the composition, the complex rheological behaviour of blood also arises from the 'clumping' of erythrocytes (red blood cells) due to the presence of fibrinogen on their surface.

The Casson model can be used to describe blood rheology. It can be stated as

$$\tau^{1/2} = \tau_0^{1/2} + \mu^{1/2} \left| \frac{-dv_x}{dy} \right|^{1/2} \tag{3.1-6}$$

where τ_0 is the yield stress.

The yield stress depends on the volume fraction of erythrocytes in the blood. The volume fraction of erythrocytes in blood is usually referred to as the 'hematocrit' and has a typical value of 0.4.

At lower shear rates, say $< 20\ \mathrm{s}^{-1}$, blood shows a complex behaviour that necessitates the use of Eq. 3.1-6, whereas at higher shear rates, say $> 100\ \mathrm{s}^{-1}$, blood can be assumed, without loss in accuracy, to behave as a Newtonian fluid. Blood rheology is highly complex and a lot of work has been done on this aspect alone so much so that an entire field of study – hemorheology – is dedicated to it.

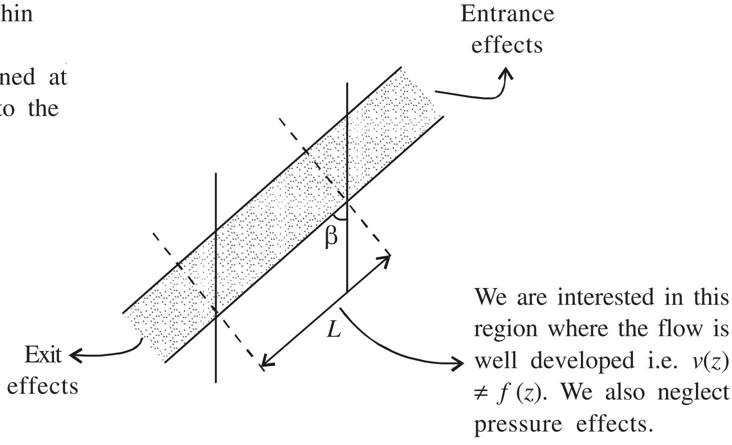
3.2 Types of Flows

Osborne Reynolds studied flows at various flow rates and found that the nature of flow changes with flow rate. Through his now classic, flow visualisation experiment (Reynolds 1883), Reynolds reported that at low flow rates, the flow in a pipe is in layers or laminae, and hence can be called 'laminar flow'. Above a certain flow rate, the flow becomes chaotic, and is called 'turbulent flow'. There is a range of flow rates where one cannot say beforehand whether the flow would be 'laminar' or 'turbulent'. This range/region is called the 'transition region'.

A non-dimensional number, called the Reynolds number, can be used to predict whether the flow will be laminar or turbulent. The Reynolds number is defined as

$$N_{\mathrm{Re}} = \frac{\rho v d}{\mu} \tag{3.2-1}$$

Fig. 3.3-1 Thin flow over a surface inclined at an angle β to the vertical



where ρ is density of the fluid, v is velocity of the fluid, d is pipe diameter and μ is viscosity of the fluid.

In pipe flow (*and only in pipe flow*), the following numbers hold:

$N_{\mathrm{Re}} < 2100$	Laminar flow
$2100 < N_{\mathrm{Re}} < 4000$	Transition
$N_{\mathrm{Re}} > 4000$	Turbulent flow

In the initial part of this chapter, we will deal with laminar flow, and then explicitly address ways to deal with turbulent flows.

3.3 Shell Momentum Balances

Since momentum is a conserved quantity, momentum balance can be used as a principle to obtain useful relationships. In this section, let us do momentum balances over a thin shell of fluid. In other words, the thin shell is the 'system' or 'control volume' over which the momentum balance is written. This technique for solving relevant problems is called the 'shell balance' technique.

To illustrate the technique, let us consider the case of flow in a falling film over an inclined surface (Fig. 3.3-1). Characteristics of such flow are used to evaluate the rheological properties of biological solutions. For example, the 'Bostwick viscometer' is based on the principle of flow over an inclined surface.

We know from basic physics that momentum is a conserved quantity in the absence of external forces. When external forces are present, according

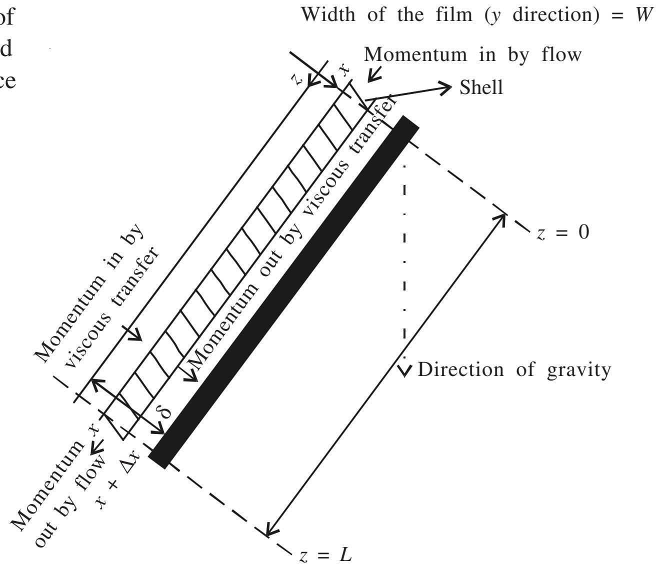


Fig. 3.3-2 Details of the shell considered for the shell balance

to Newton's second law, the rate of change of momentum is equal to the (vector) sum of the forces that act on the system or the control volume, in the direction of motion. In the case of a balance on the total mass, we could write

$$\begin{pmatrix}\text{Rate of total mass}\\ \text{out of the system}\end{pmatrix}-\begin{pmatrix}\text{Rate of total mass}\\ \text{into the system}\end{pmatrix}+\begin{pmatrix}\text{Rate of total mass}\\ \text{accumulation in the system}\end{pmatrix}=0$$

For a system (or a control volume) that has momentum being brought into it and taken out of it by flowing streams (by convection), a useful form of Newton's second law can be written as

$$\begin{pmatrix}\text{Rate of momentum}\\ \text{out of the system}\end{pmatrix}-\begin{pmatrix}\text{Rate of momentum}\\ \text{into the system}\end{pmatrix}$$
$$+\begin{pmatrix}\text{Rate of momentum}\\ \text{accumulation in the system}\end{pmatrix}=\begin{pmatrix}\text{Sum of forces acting}\\ \text{on the system}\end{pmatrix} \tag{3.3-1}$$

At steady state, the accumulation rate can be set to zero, and the balance becomes

$$\begin{pmatrix}\text{Rate of momentum}\\ \text{into the system}\end{pmatrix}-\begin{pmatrix}\text{Rate of momentum}\\ \text{out of the system}\end{pmatrix}+\begin{pmatrix}\text{Sum of forces acting}\\ \text{on the system}\end{pmatrix}=0$$

Momentum can enter the shell (system) by: (i) molecular means (momentum flux) and/or (ii) convection (bulk fluid motion), as illustrated in Fig. 3.3-2.

Further, there could be many forces that act on the system. For illustration, let us consider only the gravity forces that act on the whole volume. The pressure force and the normal force may not be relevant to the direction considered.

We are interested in $v_z(x)$ and $\tau_{xz}(x)$. Let us first acknowledge that the rate of momentum is area × momentum flux.

By Molecular Mechanism

Rate of z momentum in, across the surface at x: $(LW)\ \tau_{xz}|_x$
Rate of z momentum out, across the surface at $x + \Delta x$: $(LW)\ \tau_{xz}|_{x+\Delta x}$

By Convection

Rate of z momentum in, across the surface at $z = 0$: $(W\ \Delta x\ v_z)\ (\rho v_z)|_{z=0}$
Rate of z momentum out, across the surface at $z = L$: $(W\ \Delta x\ v_z)\ (\rho v_z)|_{z=L}$
Gravity force acting on the fluid in the direction of motion: $(L\ W\ \Delta x)\ (\rho\ g \cos\beta)$

Substituting the above in the momentum balance, Eq. 3.3-1, at steady state, we get

$$LW\,\tau_{xz}\big|_x - LW\,\tau_{xz}\big|_{x+\Delta x} + W\,\Delta x\,\rho\,v_z^2\big|_{z=0} - W\,\Delta x\,\rho\,v_z^2\big|_{z=L} + LW\,\Delta x\,\rho\,g\cos\beta = 0 \tag{3.3-2}$$

Since we have chosen conditions such that $v_z \neq f(z)$, the third and fourth terms on the LHS cancel each other. Then, if we divide the equation by $LW\Delta x$ and take the limit as $\Delta x \to 0$

$$\lim_{\Delta x \to 0}\left(\frac{\tau_{xz}\big|_{x+\Delta x} - \tau_{xz}\big|_x}{\Delta x}\right) = \rho\,g\cos\beta$$

i.e.

$$\frac{d\tau_{xz}}{dx} = \rho\,g\cos\beta \tag{3.3-3}$$

The solution of the above first order differential equation (DE) is

$$\tau_{xz} = \rho\ g\ x\ \cos\beta + C_1 \tag{3.3-4}$$

To evaluate C_1, we need a boundary condition.

Notice that $x = 0$ is the liquid-gas interface. A standard boundary condition that can be used at *liquid-gas interfaces* is that the momentum flux (hence the velocity gradient) in the liquid phase can be assumed to be zero for most calculations. i.e.

$$\text{at } x = 0,\ \tau_{xz} = 0 \tag{3.3-5}$$

This boundary condition applied on to the solution given in Eq. 3.3-4 yields, $C_1 = 0$. Thus

$$\tau_{xz} = \rho\ g\ x\ \cos\beta \tag{3.3-6}$$

Thus, we have the shear stress distribution, i.e. $\tau_{xz} = f\ (x)$.

To obtain the velocity distribution from the shear stress distribution, we need a link between the two. That link is conveniently provided by the constitutive equation. For example, if the fluid is Newtonian, we know that

$$\tau_{xz} = -\mu \frac{dv_z}{dx}$$

By substituting the constitutive equation in Eq. 3.3-6, we get

$$\frac{dv_z}{dx} = -\left(\frac{\rho\, g \cos\beta}{\mu}\right)x \tag{3.3-7}$$

The solution of the above DE is

$$v_z = -\left(\frac{\rho\, g \cos\beta}{2\mu}\right)x^2 + C_2 \tag{3.3-8}$$

C_2 can be found by another standard boundary condition – at the solid-fluid interface, the fluid velocity equals the velocity with which the surface itself is moving. It is assumed that the fluid will cling to any solid surface with which it is in contact.

Therefore

$$\text{at } x = \delta,\ v_z = 0 \tag{3.3-9}$$

By substituting the boundary condition into the solution, Eq. 3.3-8, we get

$$C_2 = \left(\frac{\rho\, g \cos\beta}{2\mu}\right)\delta^2$$

Therefore

$$v_z = \frac{\rho\, g\, \delta^2 \cos\beta}{2\mu}\left[1 - \left(\frac{x}{\delta}\right)^2\right] \tag{3.3-10}$$

It can be seen that the maximum velocity occurs at $x = 0$. Therefore

$$v_{z,\max} = \frac{\rho g \delta^2 \cos\beta}{2\mu} \tag{3.3-11}$$

Now, the average velocity over a cross-section of a film can be computed using

$$v_{z,\,\mathrm{avg}} = \frac{\int_0^w \int_0^\delta v_z dxdy}{\int_0^w \int_0^\delta dxdy} = \frac{1}{\delta}\int_0^\delta v_z dx \tag{3.3-12}$$

(since W can be cancelled in the numerator and the denominator). By substituting Eq. 3.3-10 in Eq. 3.3-12, we get

$$\begin{aligned} v_{z,\,\mathrm{avg}} &= \frac{\rho g \delta^2 \cos\beta}{2\mu}\int_0^1 \left[1-\left(\frac{x}{\delta}\right)^2\right] d\left(\frac{x}{\delta}\right) \\ &= \frac{\rho g \delta^2 \cos\beta}{2\mu}\left[\left(\frac{x}{\delta}\right)-\frac{1}{3}\left(\frac{x}{\delta}\right)^3\right]_0^1 \\ &= \frac{\rho g \delta^2 \cos\beta}{3\mu} \end{aligned} \tag{3.3-13}$$

The volume flow rate Q is given by

$$Q = \int_0^w \int_0^\delta v_z dxdy = W\delta v_{z,\,\mathrm{avg}} = W\delta \frac{\rho g \delta^2 \cos\beta}{3\mu} \tag{3.3-14}$$

3.4 Equation of Motion

Let us consider doing momentum balance in three dimensions with the realisation that momentum is a vector. To do that, let us first consider Cartesian coordinates and take the same cuboidal element that we considered for mass balance (Fig. 3.4-1).

As seen earlier, momentum flows into and out of the volume element by two means:

- convection (by virtue of bulk fluid flow)
- molecular aspects (by virtue of velocity gradients)

Fig. 3.4-1 Control volume (system) to consider for momentum balances

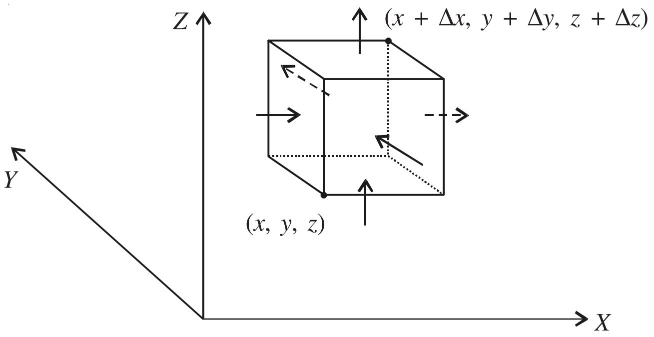
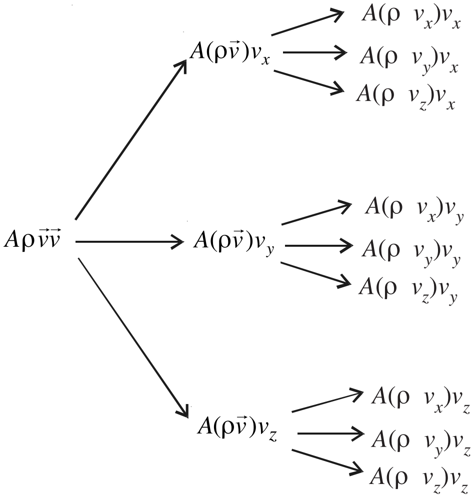


Fig. 3.4-2 The various components of the momentum rate



Momentum Rate by Convection

For momentum transport by convection, note that $(\rho\vec{v})\vec{v}$ is momentum flux (the units can be written down and checked). Thus, the rate of momentum (momentum per time) is $A(\rho\vec{v})\vec{v}$, where A is the area. The units work out as $\cancel{\mathrm{m}}^2\left(\frac{\mathrm{kg}}{\cancel{\mathrm{m}}^3}\frac{\mathrm{m}}{\mathrm{s}}\right)\frac{\cancel{\mathrm{m}}}{\mathrm{s}}$.

There are three components to the rate of momentum: x, y, and z. Each of these components is, in turn, composed of three other components, as shown in Fig. 3.4-2.

Now, let us consider only the *x component* of the momentum rate due to convection:

Entry Rates
x direction (through the face at x) = $(\rho v_x)v_x|_x\ \Delta y\Delta z$
y direction (through the face at y) = $(\rho v_y)v_x|_y\ \Delta x\Delta z$
z direction (through the face at z) = $(\rho v_z)v_x|_z\ \Delta x\Delta y$

Exit Rates
x direction (through the face at $x + \Delta x$) = $(\rho v_x)v_x|_{x+\Delta x}\ \Delta y\Delta z$
y direction (through the face at $y + \Delta y$) = $(\rho v_y)v_x|_{y+\Delta y}\ \Delta x\Delta z$
z direction (through the face at $z + \Delta z$) = $(\rho v_z)v_x|_{z+\Delta z}\ \Delta x\Delta y$

Thus, the net x momentum rate due to convection is

$$\Delta y\Delta z[(\rho v_x)v_x|_x - (\rho v_x)v_x|_{x+\Delta x}] + \Delta x\Delta z[(\rho v_y)v_x|_y - (\rho v_y)v_x|_{y+\Delta y}] \\ + \Delta x\Delta y[(\rho v_z)v_x|_z - (\rho v_z)v_x|_{z+\Delta z}]$$

Momentum Rate by Molecular Aspects

Now, let us look at the momentum rate through molecular aspects. It can be recalled, from earlier in this chapter, that shear stress is momentum flux. Thus, area × shear stress will provide an expression for the momentum rate through molecular aspects.

To begin, let us consider the force that causes the shear stress. Say that the force that acts on the face at x (refer to Fig. 3.4-1) is $\overrightarrow{F^s}_x$, the force that acts on the face at y is $\overrightarrow{F^s}_y$, and the force that acts on the face at z is $\overrightarrow{F^s}_z$. Each of these forces would have three (x, y and z) components, and the components are detailed below:

$$\left.\begin{array}{l} F^S{}_{xx} \\ F^S{}_{xy} \\ F^S{}_{xz} \end{array}\right\} \text{components of } \overrightarrow{F^S}_x$$

$$\left.\begin{matrix} F^S{}_{yx} \\ F^S{}_{yy} \\ F^S{}_{yz} \end{matrix}\right\} \text{components of } \overrightarrow{F^S}{}_y$$

$$\left.\begin{matrix} F^S{}_{zx} \\ F^S{}_{zy} \\ F^S{}_{zz} \end{matrix}\right\} \text{components of } \overrightarrow{F^S}{}_z$$

Now, let us divide the force components by the appropriate areas to get the components of the stresses.

$$\left.\begin{matrix} \tau_{xx} \\ \tau_{xy} \\ \tau_{xz} \end{matrix}\right\} \text{components of } \vec{\tau}_x$$

$$\left.\begin{matrix} \tau_{yx} \\ \tau_{yy} \\ \tau_{yz} \end{matrix}\right\} \text{components of } \vec{\tau}_y$$

$$\left.\begin{matrix} \tau_{zx} \\ \tau_{zy} \\ \tau_{zz} \end{matrix}\right\} \text{components of } \vec{\tau}_z$$

τ_{ij} denotes shear stress when $i \neq j$, and normal stress when $i = j$; both shear stress and normal stress arise due to molecular aspects.

Let us first consider only the x *component* of momentum rate due to molecular aspects.

Entry Rates
x direction = $\tau_{xx}|_x \Delta y \Delta z$
y direction = $\tau_{yx}|_y \Delta x \Delta z$
z direction = $\tau_{zx}|_z \Delta x \Delta y$

Exit Rates
x direction = $\tau_{xx}|_{x+\Delta x} \Delta y \Delta z$
y direction = $\tau_{yx}|_{y+\Delta y} \Delta x \Delta z$
z direction = $\tau_{zx}|_{z+\Delta z} \Delta x \Delta y$

Thus, the net x momentum rate due to molecular aspects is

$$\Delta y\Delta z[\tau_{xx}|_x - \tau_{xx}|_{x+\Delta x}] + \Delta x\Delta z[\tau_{yx}|_y - \tau_{yx}|_{y+\Delta y}] + \Delta x\Delta y[\tau_{zx}|_z - \tau_{zx}|_{z+\Delta z}]$$

Forces

Let us consider two important forces that usually act on the volume element, namely fluid pressure force and gravity. If there are other forces acting on the volume element, we need to consider them as additive terms in each direction.

The resultant force in the x direction is

$$\Delta y\Delta z(p|_x - p|_{x+\Delta x}) + \rho g_x\Delta x\Delta y\Delta z$$

where $p = f(\rho, T)$.

Accumulation

The accumulation of the x momentum within the volume element is

$$\Delta x\Delta y\Delta z\left(\frac{\partial \rho v_x}{\partial t}\right)$$

If we substitute the above terms for the x direction in the general momentum balance equation Eq. 3.3-1, divide by $\Delta x\Delta y\Delta z$, and take the limit as Δx, Δy, and $\Delta z \to 0$, we get

$$\frac{\partial(\rho v_x)}{\partial t} = -\left(\frac{\partial(\rho v_x v_x)}{\partial x} + \frac{\partial(\rho v_y v_x)}{\partial y} + \frac{\partial(\rho v_z v_x)}{\partial z}\right) - \left(\frac{\partial \tau_{xx}}{\partial x} + \frac{\partial \tau_{yx}}{\partial y} + \frac{\partial \tau_{zx}}{\partial z}\right) - \frac{\partial p}{\partial x} + \rho g_x \tag{3.4-1}$$

A similar exercise in the y and z directions would give

$$\frac{\partial(\rho v_y)}{\partial t} = -\left(\frac{\partial(\rho v_x v_y)}{\partial x} + \frac{\partial(\rho v_y v_y)}{\partial y} + \frac{\partial(\rho v_z v_y)}{\partial z}\right) - \left(\frac{\partial \tau_{xy}}{\partial x} + \frac{\partial \tau_{yy}}{\partial y} + \frac{\partial \tau_{zy}}{\partial z}\right) - \frac{\partial p}{\partial y} + \rho g_y \tag{3.4-2}$$

$$\frac{\partial(\rho v_z)}{\partial t} = -\left(\frac{\partial(\rho v_x v_z)}{\partial x} + \frac{\partial(\rho v_y v_z)}{\partial y} + \frac{\partial(\rho v_z v_z)}{\partial z}\right) - \left(\frac{\partial \tau_{xz}}{\partial x} + \frac{\partial \tau_{yz}}{\partial y} + \frac{\partial \tau_{zz}}{\partial z}\right) - \frac{\partial p}{\partial z} + \rho g_z \tag{3.4-3}$$

In compact, vectorial notation

$\dfrac{\partial(\rho\vec{v})}{\partial t}$	$= -[\vec{\nabla}.\rho\vec{v}\vec{v}]$	$-[\vec{\nabla}.\tilde{\tau}]$	$-\vec{\nabla}p$	$+\rho\vec{g}$
Rate of increase in momentum per unit volume	Rate of gain in momentum by convection per unit volume	Rate of gain in momentum by viscous effects per unit volume	Pressure force on the element per unit volume	Gravitational force on the element per unit volume

(3.4-4)

There are a couple of terms in Eq. 3.4-4 that could be new. A review of Eqs. 3.4-1, 3.4-2 and 3.4-3 will reveal that $\tilde{\tau}$ has 9 terms. τ is a second order tensor with 9 components that can be represented by

$$\tilde{\tau} = \begin{pmatrix} \tau_{xx} & \tau_{xy} & \tau_{xz} \\ \tau_{yx} & \tau_{yy} & \tau_{yz} \\ \tau_{zx} & \tau_{zy} & \tau_{zz} \end{pmatrix}$$

See Appendix 1 for more on tensor algebra.

Similarly, $\vec{v}\vec{v}$ is a new concept. Note that it is neither a dot product nor a cross product. A review of Eqs. 3.4-1 to 3.4-3 (first terms on the LHS) will reveal that $\vec{v}\vec{v}$ has 9 terms. $\vec{v}\vec{v}$ is known as the 'dyadic product' and is a special form of second order tensor. The dyadic product of two vectors $\vec{v}$ and $\vec{w}$ is

$$\vec{v}\vec{w} = \begin{pmatrix} v_x w_x & v_x w_y & v_x w_z \\ v_y w_x & v_y w_y & v_y w_z \\ v_z w_x & v_z w_y & v_z w_z \end{pmatrix}$$

See Appendix 1 for more on dyad algebra.

Now, let us consider Eq. 3.4-1 written as

$$\frac{\partial(\rho v_x)}{\partial t} + \left(\frac{\partial(\rho v_x v_x)}{\partial x} + \frac{\partial(\rho v_y v_x)}{\partial y} + \frac{\partial(\rho v_z v_x)}{\partial z} \right) = -\left(\frac{\partial \tau_{xx}}{\partial x} + \frac{\partial \tau_{yx}}{\partial y} + \frac{\partial \tau_{zx}}{\partial z} \right) - \frac{\partial p}{\partial x} + \rho g_x$$

The LHS can be expanded as

$$\rho\frac{\partial v_x}{\partial t} + v_x\frac{\partial \rho}{\partial t} + \left(\rho v_x\frac{\partial v_x}{\partial x} + v_x\frac{\partial \rho v_x}{\partial x} + \rho v_y\frac{\partial v_x}{\partial y} + v_x\frac{\partial \rho v_y}{\partial y} + \rho v_z\frac{\partial v_x}{\partial z} + v_x\frac{\partial \rho v_z}{\partial z} \right)$$

$$= \rho\frac{\partial v_x}{\partial t} + v_x\frac{\partial \rho}{\partial t} + v_x\left(\frac{\partial \rho v_x}{\partial x} + \frac{\partial \rho v_y}{\partial y} + \frac{\partial \rho v_z}{\partial z} \right) + \left(\rho v_x\frac{\partial v_x}{\partial x} + \rho v_y\frac{\partial v_y}{\partial y} + \rho v_z\frac{\partial v_x}{\partial z} \right)$$

$$= \rho \frac{\partial v_x}{\partial t} + v_x \frac{\partial \rho}{\partial t} + v_x \left(\rho \frac{\partial v_x}{\partial x} + v_x \frac{\partial \rho}{\partial x} + \rho \frac{\partial v_y}{\partial y} + v_y \frac{\partial \rho}{\partial y} + \rho \frac{\partial v_z}{\partial z} + v_z \frac{\partial \rho}{\partial z} \right)$$

$$+ \rho \left(v_x \frac{\partial v_x}{\partial x} + v_y \frac{\partial v_y}{\partial y} + v_z \frac{\partial v_z}{\partial z} \right)$$

$$= \left\{ v_x \frac{\partial \rho}{\partial t} + \rho v_x \left(\frac{\partial v_x}{\partial x} + \frac{\partial v_y}{\partial y} + \frac{\partial v_z}{\partial z} \right) + v_x \left(v_x \frac{\partial \rho}{\partial x} + v_y \frac{\partial \rho}{\partial y} + v_z \frac{\partial \rho}{\partial z} \right) \right\}$$

$$+ \rho \left(\frac{\partial v_x}{\partial t} + v_x \frac{\partial v_x}{\partial x} + v_y \frac{\partial v_y}{\partial y} + v_z \frac{\partial v_x}{\partial z} \right)$$

$$= \{E\} + \rho \frac{D v_x}{Dt}$$

where

$$E = v_x \left(\frac{\partial \rho}{\partial t} + v_x \frac{\partial \rho}{\partial x} + v_y \frac{\partial \rho}{\partial y} + v_z \frac{\partial \rho}{\partial z} \right) + \rho v_x \left(\frac{\partial v_x}{\partial x} + \frac{\partial v_y}{\partial y} + \frac{\partial v_z}{\partial z} \right)$$

Using the equation of continuity, Eq. 1.4.3-6, the first term on the RHS of the equation above can be written as the negative of the second term on the RHS. Thus

$$E = v_x \left[-\rho \left(\frac{\partial v_x}{\partial x} + \frac{\partial v_y}{\partial y} + \frac{\partial v_z}{\partial z} \right) \right] + \rho v_x \left(\frac{\partial v_x}{\partial x} + \frac{\partial v_y}{\partial y} + \frac{\partial v_z}{\partial z} \right) = 0$$

Thus, Eq. 3.4-1 can be written as

$$\rho \frac{D v_x}{Dt} = -\left(\frac{\partial \tau_{xx}}{\partial x} + \frac{\partial \tau_{yx}}{\partial y} + \frac{\partial \tau_{zx}}{\partial z} \right) - \frac{\partial p}{\partial x} + \rho\, g_x$$

The other two components (y and z) of momentum rate can be similarly expressed and added together, to get a 3-D representation

$\rho \frac{D\vec{v}}{Dt}$	$=$	$-[\vec{\nabla} . \tilde{\tau}]$	$-\vec{\nabla} p$	$+\rho \vec{g}$
$\frac{\text{Mass}}{\text{Volume}} \times \text{Acceleration}$		Viscous forces on the element per unit volume	Pressure force on the element per unit volume	Gravitational force on the element per unit volume

(3.4-5)

Table 3.4-1 The equations of motion in rectangular Cartesian coordinates

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x direction

$$\rho\left(\frac{\partial v_x}{\partial t}+v_x\frac{\partial v_x}{\partial x}+v_y\frac{\partial v_x}{\partial y}+v_z\frac{\partial v_x}{\partial z}\right)=-\frac{\partial p}{\partial x}-\left(\frac{\partial \tau_{xx}}{\partial x}+\frac{\partial \tau_{yx}}{\partial y}+\frac{\partial \tau_{zx}}{\partial z}\right)+\rho g_x \tag{A1}$$

For a Newtonian fluid with constant ρ and μ

$$\rho\left(\frac{\partial v_x}{\partial t}+v_x\frac{\partial v_x}{\partial x}+v_y\frac{\partial v_x}{\partial y}+v_z\frac{\partial v_x}{\partial z}\right)=-\frac{\partial p}{\partial x}+\mu\left(\frac{\partial^2 v_x}{\partial x^2}+\frac{\partial^2 v_x}{\partial y^2}+\frac{\partial^2 v_x}{\partial z^2}\right)+\rho g_x \tag{A2}$$

y direction

$$\rho\left(\frac{\partial v_y}{\partial t}+v_x\frac{\partial v_y}{\partial x}+v_y\frac{\partial v_y}{\partial y}+v_z\frac{\partial v_y}{\partial z}\right)=-\frac{\partial p}{\partial y}-\left(\frac{\partial \tau_{xy}}{\partial x}+\frac{\partial \tau_{yy}}{\partial y}+\frac{\partial \tau_{zy}}{\partial z}\right)+\rho g_y \tag{B1}$$

For a Newtonian fluid with constant ρ and μ

$$\rho\left(\frac{\partial v_y}{\partial t}+v_x\frac{\partial v_y}{\partial x}+v_y\frac{\partial v_y}{\partial y}+v_z\frac{\partial v_y}{\partial z}\right)=-\frac{\partial p}{\partial y}+\mu\left(\frac{\partial^2 v_y}{\partial x^2}+\frac{\partial^2 v_y}{\partial y^2}+\frac{\partial^2 v_y}{\partial z^2}\right)+\rho g_y \tag{B2}$$

z direction

$$\rho\left(\frac{\partial v_z}{\partial t}+v_x\frac{\partial v_z}{\partial x}+v_y\frac{\partial v_z}{\partial y}+v_z\frac{\partial v_z}{\partial z}\right)=-\frac{\partial p}{\partial z}-\left(\frac{\partial \tau_{xz}}{\partial x}+\frac{\partial \tau_{yz}}{\partial y}+\frac{\partial \tau_{zz}}{\partial z}\right)+\rho g_z \tag{C1}$$

For a Newtonian fluid with constant ρ and μ

$$\rho\left(\frac{\partial v_z}{\partial t}+v_x\frac{\partial v_z}{\partial x}+v_y\frac{\partial v_z}{\partial y}+v_z\frac{\partial v_z}{\partial z}\right)=-\frac{\partial p}{\partial z}+\mu\left(\frac{\partial^2 v_z}{\partial x^2}+\frac{\partial^2 v_z}{\partial y^2}+\frac{\partial^2 v_z}{\partial z^2}\right)+\rho g_z \tag{C2}$$

The components of Eq. 3.4-5, in different coordinate systems are given in Tables 3.4-1 to 3.4-3; the order of the first two terms on the RHS of Eq. 3.4-5 has been reversed in the tables. To determine velocity distributions and to derive further useful expressions, we need to represent the stresses in terms of velocity gradients and fluid properties. The equations in Tables 3.4-4 to 3.4-6, which give the components of the stress tensor for a Newtonian fluid in the three coordinate systems, can be used toward this objective.

Substituting the expressions from Table 3.4-4 in the momentum balances for the three directions, we get

$$\begin{aligned}\rho\frac{Dv_x}{Dt}&=\frac{\partial}{\partial x}\left[2\mu\frac{\partial v_x}{\partial x}-\frac{2}{3}\mu(\vec{\nabla}.\vec{v})\right]+\frac{\partial}{\partial y}\left[\mu\left(\frac{\partial v_x}{\partial y}+\frac{\partial v_y}{\partial x}\right)\right]\\&\quad+\frac{\partial}{\partial z}\left[\mu\left(\frac{\partial v_z}{\partial x}+\frac{\partial v_x}{\partial z}\right)\right]-\frac{\partial p}{\partial x}+\rho g_x\end{aligned} \tag{3.4-6}$$

Table 3.4-2 The equations of motion in cylindrical coordinates

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r direction

$$\rho\left(\frac{\partial v_r}{\partial t}+v_r\frac{\partial v_r}{\partial r}+\frac{v_\theta}{r}\frac{\partial v_r}{\partial \theta}-\frac{v_\theta^2}{r}+v_z\frac{\partial v_r}{\partial z}\right)=$$

$$-\frac{\partial p}{\partial r}-\left(\frac{1}{r}\frac{\partial}{\partial r}(r\tau_{rr})+\frac{1}{r}\frac{\partial \tau_{r\theta}}{\partial \theta}-\frac{\tau_{\theta\theta}}{r}+\frac{\partial \tau_{rz}}{\partial z}\right)+\rho g_r \qquad \text{(A1)}$$

For a Newtonian fluid with constant ρ and μ

$$\rho\left(\frac{\partial v_r}{\partial t}+v_r\frac{\partial v_r}{\partial r}+\frac{v_\theta}{r}\frac{\partial v_r}{\partial \theta}-\frac{v_\theta^2}{r}+v_z\frac{\partial v_r}{\partial z}\right)=$$

$$-\frac{\partial p}{\partial r}+\mu\left(\frac{\partial}{\partial r}\left(\frac{1}{r}\frac{\partial}{\partial r}(rv_r)\right)+\frac{1}{r^2}\frac{\partial^2 v_r}{\partial \theta^2}-\frac{2}{r^2}\frac{\partial v_\theta}{\partial \theta}+\frac{\partial^2 v_r}{\partial z^2}\right)+\rho g_r \qquad \text{(A2)}$$

θ direction

$$\rho\left(\frac{\partial v_\theta}{\partial t}+v_r\frac{\partial v_\theta}{\partial r}+\frac{v_\theta}{r}\frac{\partial v_\theta}{\partial \theta}+\frac{v_r v_\theta}{r}+v_z\frac{\partial v_\theta}{\partial z}\right)=$$

$$-\frac{1}{r}\frac{\partial p}{\partial \theta}-\left(\frac{1}{r^2}\frac{\partial}{\partial r}(r^2\tau_{r\theta})+\frac{1}{r}\frac{\partial \tau_{\theta\theta}}{\partial \theta}+\frac{\partial \tau_{\theta z}}{\partial z}\right)+\rho g_\theta \qquad \text{(B1)}$$

For a Newtonian fluid with constant ρ and μ

$$\rho\left(\frac{\partial v_\theta}{\partial t}+v_r\frac{\partial v_\theta}{\partial r}+\frac{v_\theta}{r}\frac{\partial v_\theta}{\partial \theta}+\frac{v_r v_\theta}{r}+v_z\frac{\partial v_\theta}{\partial z}\right)=$$

$$-\frac{1}{r}\frac{\partial p}{\partial \theta}+\mu\left(\frac{\partial}{\partial r}\left(\frac{1}{r}\frac{\partial}{\partial r}(rv_\theta)\right)+\frac{1}{r^2}\frac{\partial^2 v_\theta}{\partial \theta^2}+\frac{2}{r^2}\frac{\partial v_r}{\partial \theta}+\frac{\partial^2 v_\theta}{\partial z^2}\right)+\rho g_\theta \qquad \text{(B2)}$$

z direction

$$\rho\left(\frac{\partial v_z}{\partial t}+v_r\frac{\partial v_z}{\partial r}+\frac{v_\theta}{r}\frac{\partial v_z}{\partial \theta}+v_z\frac{\partial v_z}{\partial z}\right)=$$

$$-\frac{\partial p}{\partial z}-\left(\frac{1}{r}\frac{\partial}{\partial r}(r\tau_{rz})+\frac{1}{r}\frac{\partial \tau_{\theta z}}{\partial \theta}+\frac{\partial \tau_{zz}}{\partial z}\right)+\rho g_z \qquad \text{(C1)}$$

For a Newtonian fluid with constant ρ and μ

$$\rho\left(\frac{\partial v_z}{\partial t}+v_r\frac{\partial v_z}{\partial r}+\frac{v_\theta}{r}\frac{\partial v_z}{\partial \theta}+v_z\frac{\partial v_z}{\partial z}\right)=$$

$$-\frac{\partial p}{\partial z}+\mu\left(\frac{1}{r}\frac{\partial}{\partial r}\left(r\frac{\partial v_z}{\partial r}\right)+\frac{1}{r^2}\frac{\partial^2 v_z}{\partial \theta^2}+\frac{\partial^2 v_z}{\partial z^2}\right)+\rho g_z \qquad \text{(C2)}$$

Table 3.4-3 The equations of motion in spherical coordinates*

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r direction

$$\rho\left(\frac{\partial v_r}{\partial t}+v_r\frac{\partial v_r}{\partial r}+\frac{v_\theta}{r}\frac{\partial v_r}{\partial\theta}+\frac{v_\phi}{r\sin\theta}\frac{\partial v_r}{\partial\phi}-\frac{v_\theta^2+v_\phi^2}{r}\right)=-\frac{\partial p}{\partial r}$$

$$-\left(\frac{1}{r^2}\frac{\partial}{\partial r}(r^2\tau_{rr})+\frac{1}{r\sin\theta}\frac{\partial(\tau_{r\theta}\sin\theta)}{\partial\theta}+\frac{1}{r\sin\theta}\frac{\partial\tau_{r\theta}}{\partial\phi}-\frac{\tau_{\theta\theta}+\tau_{\phi\phi}}{r}\right)+\rho g_r \qquad \text{(A1)}$$

For a Newtonian fluid with constant ρ and μ

$$\rho\left(\frac{\partial v_r}{\partial t}+v_r\frac{\partial v_r}{\partial r}+\frac{v_\theta}{r}\frac{\partial v_r}{\partial\theta}+\frac{v_\phi}{r\sin\theta}\frac{\partial v_r}{\partial\phi}-\frac{v_\theta^2+v_\phi^2}{r}\right)=-\frac{\partial p}{\partial r}$$

$$+\mu\left(\nabla^2 v_r-\frac{2}{r^2}v_r-\frac{2}{r^2}\frac{\partial v_\theta}{\partial\theta}-\frac{2}{r^2}v_\theta\cot\theta-\frac{2}{r^2\sin\theta}\frac{\partial v_\phi}{\partial\phi}\right)+\rho g_r \qquad \text{(A2)}$$

θ direction

$$\rho\left(\frac{\partial v_\theta}{\partial t}+v_r\frac{\partial v_\theta}{\partial r}+\frac{v_\theta}{r}\frac{\partial v_\theta}{\partial\theta}+\frac{v_\phi}{r\sin\theta}\frac{\partial v_\theta}{\partial\phi}+\frac{v_r v_\theta}{r}-\frac{v_\phi^2\cot\theta}{r}\right)=-\frac{1}{r}\frac{\partial p}{\partial\theta}$$

$$-\left(\frac{1}{r^2}\frac{\partial}{\partial r}(r^2\tau_{r\theta})+\frac{1}{r\sin\theta}\frac{\partial(\tau_{\theta\theta}\sin\theta)}{\partial\theta}+\frac{1}{r\sin\theta}\frac{\partial\tau_{\theta\phi}}{\partial\phi}+\frac{\tau_{r\theta}}{r}-\frac{\cot\theta}{r}\tau_{\phi\phi}\right)+\rho g_\theta \qquad \text{(B1)}$$

For a Newtonian fluid with constant ρ and μ

$$\rho\left(\frac{\partial v_\theta}{\partial t}+v_r\frac{\partial v_\theta}{\partial r}+\frac{v_\theta}{r}\frac{\partial v_\theta}{\partial\theta}+\frac{v_\phi}{r\sin\theta}\frac{\partial v_\theta}{\partial\phi}+\frac{v_r v_\theta}{r}-\frac{v_\phi^2\cot\theta}{r}\right)=-\frac{1}{r}\frac{\partial p}{\partial\theta}$$

$$+\mu\left(\nabla^2 v_\theta+\frac{2}{r^2}\frac{\partial v_r}{\partial\theta}-\frac{v_\theta}{r^2\sin^2\theta}-\frac{2}{r^2}\frac{\cos\theta}{\sin^2\theta}\frac{\partial v_\phi}{\partial\phi}\right)+\rho g_\theta \qquad \text{(B2)}$$

ϕ direction

$$\rho\left(\frac{\partial v_\phi}{\partial t}+v_r\frac{\partial v_\phi}{\partial r}+\frac{v_\theta}{r}\frac{\partial v_\phi}{\partial\theta}+\frac{v_\phi}{r\sin\theta}\frac{\partial v_\phi}{\partial\phi}+\frac{v_\phi v_r}{r}+\frac{v_\theta v_\phi}{r}\cot\theta\right)=-\frac{1}{r\sin\theta}\frac{\partial p}{\partial\phi}$$

$$-\left(\frac{1}{r^2}\frac{\partial}{\partial r}(r^2\tau_{r\phi})+\frac{1}{r}\frac{\partial\tau_{\theta\phi}}{\partial\theta}+\frac{1}{r\sin\theta}\frac{\partial\tau_{\phi\phi}}{\partial\phi}+\frac{\tau_{r\phi}}{r}+\frac{2\cot\theta}{r}\tau_{\theta\phi}\right)+\rho g_\phi \qquad \text{(C1)}$$

For a Newtonian fluid with constant ρ and μ

$$\rho\left(\frac{\partial v_\phi}{\partial t}+v_r\frac{\partial v_\phi}{\partial r}+\frac{v_\theta}{r}\frac{\partial v_\phi}{\partial\theta}+\frac{v_\phi}{r\sin\theta}\frac{\partial v_\phi}{\partial\phi}+\frac{v_\phi v_r}{r}+\frac{v_\theta v_\phi}{r}\cot\theta\right)=-\frac{1}{r\sin\theta}\frac{\partial p}{\partial\phi}$$

$$+\mu\left(\nabla^2 v_\phi-\frac{v_\phi}{r^2\sin^2\theta}+\frac{2}{r^2\sin\theta}\frac{\partial v_r}{\partial\phi}+\frac{2\cos\theta}{r^2\sin^2\theta}\frac{\partial v_\theta}{\partial\phi}\right)+\rho g_\phi \qquad \text{(C2)}$$

---

*Note that $\nabla^2=\dfrac{1}{r^2}\dfrac{\partial}{\partial r}\left(r^2\dfrac{\partial}{\partial r}\right)+\dfrac{1}{r^2\sin\theta}\dfrac{\partial}{\partial\theta}\left(\sin\theta\dfrac{\partial}{\partial\theta}\right)+\dfrac{1}{r^2\sin^2\theta}\left(\dfrac{\partial^2}{\partial\phi^2}\right)$

Table 3.4-4 Components of the stress tensor for Newtonian fluids in rectangular Cartesian coordinates

$$\tau_{xy} = \tau_{yx} = -\mu\left(\frac{\partial v_x}{\partial y} + \frac{\partial v_y}{\partial x}\right) \qquad \text{(A)}$$

$$\tau_{yz} = \tau_{zy} = -\mu\left(\frac{\partial v_y}{\partial z} + \frac{\partial v_z}{\partial y}\right) \qquad \text{(B)}$$

$$\tau_{zx} = \tau_{xz} = -\mu\left(\frac{\partial v_z}{\partial x} + \frac{\partial v_x}{\partial z}\right) \qquad \text{(C)}$$

$$\tau_{xx} = -2\mu\frac{\partial v_x}{\partial x} + \frac{2}{3}\mu\left(\frac{\partial v_x}{\partial x} + \frac{\partial v_y}{\partial y} + \frac{\partial v_z}{\partial z}\right) \qquad \text{(D)}$$

$$\tau_{yy} = -2\mu\frac{\partial v_y}{\partial y} + \frac{2}{3}\mu\left(\frac{\partial v_x}{\partial x} + \frac{\partial v_y}{\partial y} + \frac{\partial v_z}{\partial z}\right) \qquad \text{(E)}$$

$$\tau_{zz} = -2\mu\frac{\partial v_z}{\partial z} + \frac{2}{3}\mu\left(\frac{\partial v_x}{\partial x} + \frac{\partial v_y}{\partial y} + \frac{\partial v_z}{\partial z}\right) \qquad \text{(F)}$$

Table 3.4-5 Components of the stress tensor for Newtonian fluids in cylindrical coordinates

$$\tau_{r\theta} = \tau_{\theta r} = -\mu\left(r\frac{\partial}{\partial r}\left(\frac{v_\theta}{r}\right) + \frac{1}{r}\frac{\partial v_r}{\partial \theta}\right) \qquad \text{(A)}$$

$$\tau_{\theta z} = \tau_{z\theta} = -\mu\left(\frac{\partial v_\theta}{\partial z} + \frac{1}{r}\frac{\partial v_z}{\partial \theta}\right) \qquad \text{(B)}$$

$$\tau_{zr} = \tau_{rz} = -\mu\left(\frac{\partial v_z}{\partial r} + \frac{\partial v_r}{\partial z}\right) \qquad \text{(C)}$$

$$\tau_{rr} = -2\mu\frac{\partial v_r}{\partial r} + \frac{2}{3}\mu\left(\frac{1}{r}\frac{\partial (rv_r)}{\partial r} + \frac{1}{r}\frac{\partial v_\theta}{\partial \theta} + \frac{\partial v_z}{\partial z}\right) \qquad \text{(D)}$$

$$\tau_{\theta\theta} = -2\mu\left(\frac{1}{r}\frac{\partial v_\theta}{\partial \theta} + \frac{v_r}{r}\right) + \frac{2}{3}\mu\left(\frac{1}{r}\frac{\partial (rv_r)}{\partial r} + \frac{1}{r}\frac{\partial v_\theta}{\partial \theta} + \frac{\partial v_z}{\partial z}\right) \qquad \text{(E)}$$

$$\tau_{zz} = -2\mu\frac{\partial v_z}{\partial z} + \frac{2}{3}\mu\left(\frac{1}{r}\frac{\partial (rv_r)}{\partial r} + \frac{1}{r}\frac{\partial v_\theta}{\partial \theta} + \frac{\partial v_z}{\partial z}\right) \qquad \text{(F)}$$

Table 3.4-6 Components of the stress tensor for Newtonian fluids in spherical coordinates

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$$\tau_{r\theta} = \tau_{\theta r} = -\mu\left(r\frac{\partial}{\partial r}\left(\frac{v_\theta}{r}\right) + \frac{1}{r}\frac{\partial v_r}{\partial \theta}\right) \tag{A}$$

$$\tau_{\theta\phi} = \tau_{\phi\theta} = -\mu\left(\frac{\sin\theta}{r}\frac{\partial}{\partial \theta}\left(\frac{v_\phi}{\sin\theta}\right) + \frac{1}{r\sin\theta}\frac{\partial v_\theta}{\partial \phi}\right) \tag{B}$$

$$\tau_{\phi r} = \tau_{r\phi} = -\mu\left(\frac{1}{r\sin\theta}\frac{\partial v_r}{\partial \phi} + r\frac{\partial}{\partial r}\left(\frac{v_\phi}{r}\right)\right) \tag{C}$$

$$\tau_{rr} = -2\mu\frac{\partial v_r}{\partial r} + \frac{2}{3}\mu\left(\frac{1}{r^2}\frac{\partial (r^2 v_r)}{\partial r} + \frac{1}{r\sin\theta}\frac{\partial (v_\theta \sin\theta)}{\partial \theta} + \frac{1}{r\sin\theta}\frac{\partial v_\phi}{\partial \phi}\right) \tag{D}$$

$$\tau_{\theta\theta} = -2\mu\left(\frac{1}{r}\frac{\partial v_\theta}{\partial \theta} + \frac{v_r}{r}\right) + \frac{2}{3}\mu\left(\frac{1}{r^2}\frac{\partial (r^2 v_r)}{\partial r} + \frac{1}{r\sin\theta}\frac{\partial (v_\theta \sin\theta)}{\partial \theta} + \frac{1}{r\sin\theta}\frac{\partial v_\phi}{\partial \phi}\right) \tag{E}$$

$$\begin{aligned}\tau_{\phi\phi} = {} & -2\mu\left(\frac{1}{r\sin\theta}\frac{\partial v_\phi}{\partial \phi} + \frac{v_r}{r} + \frac{v_\theta \cot\theta}{r}\right) \\ & + \frac{2}{3}\mu\left(\frac{1}{r^2}\frac{\partial (r^2 v_r)}{\partial r} + \frac{1}{r\sin\theta}\frac{\partial (v_\theta \sin\theta)}{\partial \theta} + \frac{1}{r\sin\theta}\frac{\partial v_\phi}{\partial \phi}\right)\end{aligned} \tag{F}$$

$$\begin{aligned}\rho\frac{Dv_y}{Dt} = {} & \frac{\partial}{\partial x}\left[\mu\left(\frac{\partial v_x}{\partial y} + \frac{\partial v_y}{\partial x}\right)\right] + \frac{\partial}{\partial y}\left[2\mu\frac{\partial v_y}{\partial y} - \frac{2}{3}\mu(\vec{\nabla}.\vec{v})\right] \\ & + \frac{\partial}{\partial z}\left[\mu\left(\frac{\partial v_y}{\partial z} + \frac{\partial v_z}{\partial y}\right)\right] - \frac{\partial p}{\partial y} + \rho g_y\end{aligned} \tag{3.4-7}$$

$$\begin{aligned}\rho\frac{Dv_z}{Dt} = {} & \frac{\partial}{\partial x}\left[\mu\left(\frac{\partial v_z}{\partial x} + \frac{\partial v_x}{\partial z}\right)\right] + \frac{\partial}{\partial y}\left[\mu\left(\frac{\partial v_y}{\partial z} + \frac{\partial v_z}{\partial y}\right)\right] \\ & + \frac{\partial}{\partial z}\left[2\mu\frac{\partial v_z}{\partial z} - \frac{2}{3}\mu(\vec{\nabla}.\vec{v})\right] - \frac{\partial p}{\partial z} + \rho g_z\end{aligned} \tag{3.4-8}$$

The equations of motion (Eqs. 3.4-6 to 3.4-8), equation of state, $p = f(\rho)$, and variation of $\mu = f(\rho)$ completely determine the pressure, density and velocity components in the flowing Newtonian fluid.

When ρ and μ are constant, since $\vec{\nabla}.\vec{v} = 0$ according to the continuity equation, the equation of motion can be written as

$$\rho\frac{D\vec{v}}{Dt} = \mu\vec{\nabla}^2\vec{v} - \vec{\nabla}p + \rho\vec{g} \tag{3.4-9}$$

Equation 3.4-9 is called the Navier-Stokes equation.

If viscous effects are not important, $\vec{\nabla}\,.\,\tilde{\tau} = 0$. Then, Eq. 3.4-5 becomes

$$\rho \frac{D\vec{v}}{Dt} = -\vec{\nabla} p + \rho \vec{g} \tag{3.4-10}$$

Equation 3.4-10 is called the Euler equation.

3.4.1 Applications of the Equations of Motion: Steady State Falling Film

The equations of motion given in Tables 3.4-1 to 3.4-3 can be used to solve problems more easily compared to using shell balances. Note that simpler equations are available in certain cases (e.g. for Eq. A2 in Table 3.4-3), which are given in other texts.

To illustrate this, let us solve the steady state falling film problem that we did in Section 3.3, using the equation of motion.

For convenience in this system geometry, let us use rectangular coordinates. Let us use Eq. C1 of Table 3.4-1 to get the shear stress profile. Note that $v_x = 0$, $v_y = 0$. Therefore, only Eq. C1 with v_z is relevant.

$$\rho\left(\overset{\substack{=0,\ \text{SS}\\ \uparrow}}{\cancel{\frac{\partial v_z}{\partial t}}} + \overset{\substack{=0,\\ v_x=0\\ \uparrow}}{\cancel{v_x}}\frac{\partial v_z}{\partial x} + \overset{\substack{=0,\\ v_y=0\\ \uparrow}}{\cancel{v_y}}\frac{\partial v_z}{\partial y} + v_z \overset{\substack{=0,\ v_z\ \text{is}\\ \text{not a } f(z)\\ \uparrow}}{\cancel{\frac{\partial v_z}{\partial z}}}\right) = -\overset{\substack{=0,\ \text{chosen}\\ \text{condition}\\ \uparrow}}{\cancel{\frac{\partial p}{\partial z}}} - \left(\frac{\partial \tau_{xz}}{\partial x} + \overset{\substack{=0,\ \tau_{yz}\ \text{is}\\ \text{not a } f(y)\\ \uparrow}}{\cancel{\frac{\partial \tau_{yz}}{\partial y}}} + \overset{\substack{=0,\ \tau_{zz}\ \text{is}\\ \text{not a } f(z)\\ \uparrow}}{\cancel{\frac{\partial \tau_{zz}}{\partial z}}}\right) + \rho g_z \tag{3.4.1-1}$$

Since

$$g_z = g \cos\beta$$

we get

$$0 = -\frac{\partial \tau_{xz}}{\partial x} + \rho g \cos\beta$$

which is the same equation as Eq. 3.3-3.

To get the velocity profile of a Newtonian fluid, we can directly begin from Eq. C2 of Table 3.4-1.

$$\rho\left(\overset{\substack{=0,\ \text{SS}\\ \uparrow}}{\cancel{\frac{\partial v_z}{\partial t}}} + \overset{\substack{=0,\\ v_x=0\\ \uparrow}}{\cancel{v_x}}\frac{\partial v_z}{\partial x} + \overset{\substack{=0,\\ v_y=0\\ \uparrow}}{\cancel{v_y}}\frac{\partial v_z}{\partial y} + v_z \overset{\substack{=0,\ v_z\ \text{is}\\ \text{not a } f(z)\\ \uparrow}}{\cancel{\frac{\partial v_z}{\partial z}}}\right) = -\overset{\substack{=0,\ \text{chosen}\\ \text{condition}\\ \uparrow}}{\cancel{\frac{\partial p}{\partial z}}} + \mu\left(\frac{\partial^2 v_z}{\partial x^2} + \overset{\substack{=0,\ v_z\ \text{is}\\ \text{not a } f(y)\\ \uparrow}}{\cancel{\frac{\partial^2 v_z}{\partial y^2}}} + \overset{\substack{=0,\ v_z\ \text{is}\\ \text{not a } f(z)\\ \uparrow}}{\cancel{\frac{\partial^2 v_z}{\partial z^2}}}\right) + \rho g_z$$

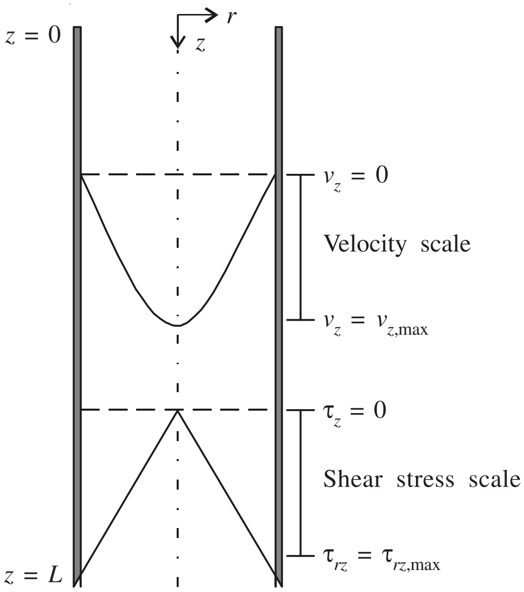


Fig. 3.4.2-1 Velocity profile and shear stress profile for a laminar flow in a cylindrical pipe

$$0 = \mu \frac{\partial^2 v_z}{\partial x^2} + \rho g \cos\beta \tag{3.4.1-2}$$

i.e.

$$\mu \frac{\partial}{\partial x}\left(\frac{\partial v_z}{\partial x}\right) = -\rho g \cos\beta$$

or

$$\frac{\partial v_z}{\partial x} = -\left(\frac{\rho g \cos\beta}{\mu}\right) x$$

which is the same equation as Eq. 3.3-7.

3.4.2 Flow in a Cylindrical Pipe

Let us consider the laminar flow through a pipe of cylindrical cross-section. The results have significance in a variety of situations ranging from flow in micro-devices, flow of body fluids in the human body, and at least as a first approximation, to the flow of liquids and gases in the bio-process industry.

Figure 3.4.2-1 shows the laminar flow of a Newtonian fluid down a cylindrical pipe placed vertically. Let the flow be well-developed, i.e. the axial velocity at any particular radial position in the pipe is not dependent on the length, $v_z \neq f(z)$.

Let us derive the profiles of shear rates and velocities across the tube diameter.

Since the system of interest is cylindrical, it is best to use cylindrical coordinates here. Thus, the Table 3.4-2 is relevant: since there is no radial flow, the r component is irrelevant. Similarly, since there is no flow around the axis of the cylinder, the θ component is irrelevant. The only relevant component is, thus, the z component.

Let us first use Eq. A2 from Table 3.4-2

$$\rho\left(\overset{\substack{(SS)\\0\\\uparrow}}{\cancel{\frac{\partial v_r}{\partial t}}} + v_r \overset{\substack{(v_r=0)\\0\\\uparrow}}{\cancel{\frac{\partial v_r}{\partial r}}} + \overset{\substack{(v_\theta=0)\\0\\\uparrow}}{\cancel{\frac{v_\theta}{r}}}\frac{\partial v_r}{\partial \theta} - \overset{\substack{(v_\theta=0)\\0\\\uparrow}}{\cancel{\frac{v_\theta^2}{r}}} + v_z \overset{\substack{(v_r \neq f(z))\\(v_r=0)\\0\\\uparrow}}{\cancel{\frac{\partial v_r}{\partial z}}}\right)$$

$$= -\frac{\partial p}{\partial r} + \mu\left[\frac{\partial}{\partial r}\left(\frac{1}{r}\frac{\partial}{\partial r}\overset{\substack{(v_r=0)\\0\\\uparrow}}{\cancel{(r v_r)}}\right) + \frac{1}{r^2}\overset{\substack{v_r \neq f(\theta)\\(v_r=0)\\0\\\uparrow}}{\cancel{\frac{\partial^2 v_r}{\partial \theta^2}}} + \frac{2}{r^2}\overset{\substack{(v_\theta=0)\\0\\\uparrow}}{\cancel{\frac{\partial v_\theta}{\partial \theta}}} + \overset{\substack{(v_r \neq f(z))\\(v_r=0)\\0\\\uparrow}}{\cancel{\frac{\partial^2 v_r}{\partial z^2}}}\right] + \overset{\substack{(g_r=0)\\0\\\uparrow}}{\cancel{\rho g_r}} \tag{3.4.2-1}$$

The equation reduces to

$$\frac{\partial p}{\partial r} = 0 \text{ or } p \neq f(r) \tag{3.4.2-2}$$

This is an important insight, i.e. the pressure across the cross-section of a pipe at a particular length in laminar flow through a pipe does not depend on the radial position.

Let us next consider Eq. B2 from Table 3.4-2

$$\rho\left(\overset{\substack{(SS)\\0\\\uparrow}}{\cancel{\frac{\partial v_\theta}{\partial t}}} + v_r \overset{\substack{(v_r=0)\\0\\\uparrow}}{\cancel{\frac{\partial v_\theta}{\partial r}}} + \overset{\substack{(v_\theta=0)\\0\\\uparrow}}{\cancel{\frac{v_\theta}{r}}}\frac{\partial v_\theta}{\partial \theta} + \overset{\substack{(v_r,\, v_\theta=0)\\0\\\uparrow}}{\cancel{\frac{v_r v_\theta}{r}}} + v_z \overset{\substack{(v_\theta \neq f(z))\\0\\\uparrow}}{\cancel{\frac{\partial v_\theta}{\partial z}}}\right)$$

$$= -\frac{1}{r}\frac{\partial p}{\partial \theta} + \mu\left[\frac{\partial}{\partial r}\left(\frac{1}{r}\frac{\partial}{\partial r}\overset{\substack{(v_\theta=0)\\0\\\uparrow}}{\cancel{(r v_\theta)}}\right) + \frac{1}{r^2}\overset{\substack{v_\theta \neq f(\theta)\\(v_\theta=0)\\0\\\uparrow}}{\cancel{\frac{\partial^2 v_\theta}{\partial \theta^2}}} + \frac{2}{r^2}\overset{\substack{v_r \neq f(\theta)\\(v_r=0)\\0\\\uparrow}}{\cancel{\frac{\partial v_r}{\partial \theta}}} + \overset{\substack{v_\theta \neq f(z)\\(v_\theta=0)\\0\\\uparrow}}{\cancel{\frac{\partial^2 v_\theta}{\partial z^2}}}\right] + \overset{\substack{(g_\theta=0)\\0\\\uparrow}}{\cancel{\rho g_\theta}} \tag{3.4.2-3}$$

The equation reduces to

$$-\frac{1}{r}\frac{\partial p}{\partial \theta}=0$$

Thus

$$\frac{\partial p}{\partial \theta}=0$$

or

$$p \neq f(\theta) \tag{3.4.2-4}$$

Thus, the pressure does not depend on the angular position in the pipe.

Now, let us consider Eq. C2 from Table 3.4-2

$$\rho\left(\overset{\substack{(\text{SS})\\0}}{\cancel{\frac{\partial v_z}{\partial t}}}+v_r\overset{\substack{(v_r=0)\\0}}{\cancel{\frac{\partial v_z}{\partial r}}}+\overset{\substack{(v_\theta=0)\\0}}{\cancel{\frac{v_\theta}{r}}}\frac{\partial v_z}{\partial \theta}+v_z\overset{\substack{(v_z\neq f(z))\\0}}{\cancel{\frac{\partial v_z}{\partial z}}}\right)$$

$$=-\frac{\partial p}{\partial z}+\mu\left[\frac{1}{r}\frac{\partial}{\partial r}\left(r\frac{\partial v_z}{\partial r}\right)+\frac{1}{r^2}\overset{\substack{v_z\neq f(\theta)\\0}}{\cancel{\frac{\partial^2 v_z}{\partial \theta^2}}}+\overset{\substack{(v_z\neq f(z))\\0}}{\cancel{\frac{\partial^2 v_z}{\partial z^2}}}\right]+\rho g_z \tag{3.4.2-5}$$

While considering the terms in the above equation, $v_z \neq f(\theta)$ because the flow, in this case, occurs in cylindrical layers. In other words, the axial velocities at all points at a particular radius, and length do not vary with θ.

$$-\frac{\mu}{r}\frac{\partial}{\partial r}\left(r\frac{\partial v_z}{\partial r}\right)=-\frac{\partial p}{\partial z}+\rho g_z \tag{3.4.2-6}$$

Let us define

$$P = p - \rho g_z z$$

Since $g_z = g$, we can write

$$\frac{\partial p}{\partial z}-\rho g=\frac{\partial(P-\rho g z)}{\partial z}=\frac{\partial P}{\partial z}$$

Therefore

$$\frac{\mu}{r}\frac{\partial}{\partial r}\left(r\frac{\partial v_z}{\partial r}\right)=\frac{\partial P}{\partial z} \tag{3.4.2-7}$$

We know from Eqs. 3.4.2-2 and 3.4.2-4 that $p \neq f(r)$ and $p \neq f(\theta)$.

Thus, $P = p + \rho g z \neq f(r)$ and $\neq f(\theta)$.

Since $p = f(z)$ alone, the partial derivative on the RHS can be replaced by an ordinary derivative.

Similarly, v_z and r are only $f(r)$; they are not $f(\theta)$ or $f(z)$. Thus the partial derivative on the LHS can also be replaced by ordinary derivative, and the equation becomes

$$\frac{\mu}{r}\frac{d}{dr}\left(r\frac{dv_z}{dr}\right)=\frac{dP}{dz} \qquad (3.4.2\text{-}8)$$

Besides, the LHS is a function of r and the RHS is a function of z, i.e.

$$\frac{\mu}{r}\frac{df(r)}{dr}=\frac{df(z)}{dz} \qquad (3.4.2\text{-}9)$$

This is possible only if each derivative equals a constant, say C_1.

Let us take the RHS of Eq. 3.4.2-8 first

$$\frac{dP}{dz}=C_1 \qquad (3.4.2\text{-}10)$$

Then

$$P = C_1 z + C_2 \qquad (3.4.2\text{-}11)$$

The relevant boundary conditions are

$$\text{At } z = 0, \quad P = P_0$$
$$\text{At } z = L, \quad P = P_L$$

Thus

$$C_2 = P_0$$

$$C_1 = \frac{P_L - P_0}{L}$$

Therefore

$$P=\left(\frac{P_L-P_0}{L}\right)z+P_0 \qquad (3.4.2\text{-}12)$$

Now let consider the LHS and equate it to the same C_1

$$\frac{\mu}{r}\frac{d}{dr}\left(r\frac{dv_z}{dr}\right)=C_1=\frac{\Delta P}{L}$$

where $\Delta P = P_L - P_0$.

Thus

$$\frac{d}{dr}\left(r\frac{dv_z}{dr}\right)=\frac{\Delta P}{L}\times\frac{r}{\mu}$$

Upon integration, we get

$$r\frac{dv_z}{dr} = \frac{\Delta P}{L}\frac{r^2}{2\mu} + C_2$$

At $r = 0$, C_2 must be equal to 0.

Therefore

$$\frac{dv_z}{dr} = \frac{\Delta P\, r}{2\mu L} \tag{3.4.2-13}$$

Integrating this, we get

$$v_z = \frac{\Delta P\, r^2}{4\mu\, L} + C_3 \tag{3.4.2-14}$$

Now, using the BC that at $r = R$, $v_z = 0$ ('no slip boundary condition')

$$C_3 = -\frac{\Delta P\, R^2}{4\mu\, L}$$

Thus

$$v_z = \frac{\Delta P}{4\mu L}(r^2 - R^2) = \frac{(-\Delta P)R^2}{4\mu L}\left[1 - \left(\frac{r}{R}\right)^2\right] \tag{3.4.2-15}$$

Therefore, the velocity profile is parabolic across the diameter, as shown in Fig. 3.4.2-1.

Note that $\Delta P = P_L - P_0$; typically, for the flow to occur, $P_L < P_0$, and thus $(-\Delta P)$ is positive.

The maximum velocity occurs at $r = 0$ (from Eq. 3.4.2-15), i.e., at the centre line (axis) of the tube.

$$v_{z,\max} = \frac{(-\Delta P)R^2}{4\mu L} \tag{3.4.2-16}$$

The average velocity across the cross-section

$$v_{z,\text{avg}} = \frac{\int_0^{2\pi}\int_0^R v_z r\,dr\,d\theta}{\int_0^{2\pi}\int_0^R r\,dr\,d\theta}$$

$$= \frac{\displaystyle\int_0^{2\pi}\int_0^R \frac{(-\Delta P)R^2}{4\mu L}\left\{1 - \left(\frac{r}{R}\right)^2\right\} r\,dr\,d\theta}{\dfrac{R^2}{2}\times 2\pi}$$

$$= \frac{(-\Delta P)R^2}{\pi R^2 \times 4\mu L}\left[\int_0^{2\pi}\int_0^R r dr d\theta - \int_0^{2\pi}\int_0^R \frac{r^2}{R^2} r dr d\theta\right]$$

$$= \frac{(-\Delta P)}{4\pi\mu L}\left\{\left[\frac{R^2}{2}\times 2\pi - \frac{r^4}{4\,R^2}\right]_0^R 2\pi\right\}$$

$$= \frac{(-\Delta P)}{4\pi\mu L}\left(\frac{R^2}{2}-\frac{R^2}{4}\right)2\pi$$

$$v_{z,\text{avg}} = \frac{(-\Delta P)\times R^2}{2\mu L\times 4} = \frac{(-\Delta P)R^2}{8\mu L} = \frac{1}{2}(v_{z,\max}) \qquad (3.4.2\text{-}17)$$

The volumetric flow rate, Q = Area × $v_{z,\text{avg}}$. Thus

$$Q = \frac{\pi R^2 \times (-\Delta P)R^2}{8\mu L} = \frac{\pi}{8\mu L}R^4(-\Delta P) \qquad (3.4.2\text{-}18)$$

Thus

$$\begin{aligned} Q \quad & \alpha\ (-\ \Delta P) \\ & \alpha\ R^4 \end{aligned}$$

If the radius is doubled at the same $(-\ \Delta P)$, the volumetric flow rate increases 16-fold.

Equation 3.4.2-18 is known as the Hagen-Poiseuille (pronounced as Pwah-zoo-yuh; here ‘oo’ is pronounced as in ‘book’) equation.

Let us now use Eq. C1 of Table 3.4-2 to derive an expression for the shear stress profile. To visualise $\tau_{\theta z}$, note that the first subscript, θ, refers to the direction of the velocity gradient, and the second subscript, z, refers to the direction of the stress or the force. If v_z is different at different θ, then $\tau_{\theta z}$ could arise. But, that is not the case here, in a laminar flow. A similar visualisation would provide $\tau_{zz} \neq f(z)$, since v_z does not vary with z for this well developed flow.

$$\rho\left(\overset{\text{(SS)}}{\cancel{\frac{\partial v_z}{\partial t}}} + v_r \overset{\substack{(v_r\,=\,0)\\0}}{\cancel{\frac{\partial v_z}{\partial r}}} + \overset{\substack{(v_\theta\,=\,0)\\0}}{\cancel{\frac{v_\theta}{r}\frac{\partial v_z}{\partial \theta}}} + v_z \overset{\substack{(v_z\,\neq\, f(z))\\0}}{\cancel{\frac{\partial v_z}{\partial z}}}\right)$$

$$= -\frac{\partial p}{\partial z} - \left[\frac{1}{r}\frac{\partial}{\partial r}(r\,\tau_{rz}) + \overset{\substack{\tau_{\theta z}\,\neq\, f(\theta)\\0}}{\cancel{\frac{1}{r}\frac{\partial \tau_{\theta z}}{\partial \theta}}} + \overset{\substack{\tau_{zz}\,\neq\\(f(z))\\0}}{\cancel{\frac{\partial \tau_{zz}}{\partial z}}}\right] + \rho g_z \qquad (3.4.2\text{-}19)$$

The terms that remain yield

$$\frac{1}{r}\left(\frac{\partial}{\partial r}(r\tau_{rz})\right) = -\frac{\partial p}{\partial z} + \rho g_z \tag{3.4.2-20}$$

If we define $P = p - \rho g_z z$, with the recognition that $g_z = g$, we can write the above equation as

$$\frac{1}{r}\left(\frac{\partial}{\partial r}(r\tau_{rz})\right) = -\frac{\partial P}{\partial z} \tag{3.4.2-21}$$

Using the same argument that we used for solving Eq. 3.4.2-7, the solution becomes

$$\tau_{rz} = -\frac{\Delta P\, r}{2L} + C' \tag{3.4.2-22}$$

B.C.: $\tau_{rz} = 0$ at $r = 0$.

Thus

$$\tau_{rz} = \left(-\frac{\Delta P}{2L}\right) r \tag{3.4.2-23}$$

The linear profile for τ_{rz} is shown in Fig. 3.4.2-1.

3.4.2.1 Capillary Flow

Flow through capillaries, i.e. tubes of very small linear dimension (radius, in the case of capillaries with circular cross-section) of the order of microns, is usually laminar. Capillary flows have great significance in microfluidics, flow through vasculature, flow through porous media, and many other situations of biological interest. Since the flow is laminar, the equations developed in the previous section are also applicable for flow through capillaries of circular cross-section.

Capillary flow arises because the force of attraction (adhesion force) between the liquid molecules and the molecules of the walls of the capillary duct are stronger than the attractive forces between the liquid molecules (cohesive forces). This causes the edges of the fluid near the capillary wall to rise, and due to cohesion, the liquid follows (or is dragged along by the stronger adhesion) as a whole, which results in the flow. We know from high/higher secondary school physics that cohesion results in a force that is usually represented as a force per unit length, or surface tension, γ. The capillary pressure due to surface tension at that point, or the meniscus, in a capillary of radius, r, is given by the appropriate simplification of the

Young-Laplace equation ($p_{st} = \gamma\left(\frac{1}{R_1}+\frac{1}{R_2}\right)$ where R_1 and R_2 are the radii of curvature (see Berg 2009) for a derivation of the Young-Laplace equation) as

$$p_{st} = \frac{2\gamma}{r}\cos\theta \qquad (3.4.2.1\text{-}1)$$

where θ is the contact angle (wetting angle) between the liquid and the capillary wall.

Note that this pressure is inversely proportional to the radius of the duct. It becomes predominant in capillaries, and provides the 'driving force' for the bulk flow of the liquid through the capillary, even if other 'driving forces' are absent. When other 'driving forces' such as those provided by a liquid column, or an external pump are present, the pressures can be added to get the total pressure difference for the flow ($-\Delta P$). For example, to obtain the flow rate in capillary flow when no other 'driving forces' for the flow are present, the use of the Hagen-Poiseuille relationship, Eq. 3.4.2-18, gives

$$Q = \frac{\pi}{8\mu L}r^4\left(\frac{2\gamma}{r}\right)\cos\theta = \frac{\pi\gamma}{4\mu L}r^3\cos\theta \qquad (3.4.2.1\text{-}2)$$

Since the flow rate is a product of the cross-sectional area and the penetration velocity, the penetration velocity (v_p) can be obtained by dividing the above equation by the cross-sectional area πr^2

$$v_p = \frac{dL}{dt} = \frac{\gamma}{4\mu L}r\cos\theta \qquad (3.4.2.1\text{-}3)$$

In microfluidic situations, the above equation can be integrated to get the position of the liquid front along the capillary as a function of time.

Capillary flow in porous media: Porous media is a term that refers to any medium that has a solid matrix with interconnected interstitial spaces, through which there is movement of some species of interest. For example, soil is a porous medium through which water, pollutants, fines, etc., can travel. Sometimes, interstitial spaces can be considered as a set of capillary tubes, and thus capillary flow through porous media is an area with wide applications.

Interestingly, many substances of biological interest can be considered as porous media. For example, any tissue, including whole organs such as liver, kidney, heart, brain, etc., can be treated as porous media because they contain cells that are dispersed, and connected voids through which nutrients, drugs and other substances travel to reach the cells. Tissue regeneration, which is used to grow artificial organs, typically happens on a scaffold, and this system can be considered a porous medium. Similarly, biological pollution treatment systems such as the trickling filter, or the matrix in which cells are immobilised in a type of bioreactor, can be treated as porous media.

To obtain the kinetics of liquid movement by capillary flow into a porous medium, the medium is typically treated as consisting of cylindrical capillary tubes. Then, the distance penetrated by the liquid into the porous medium L can be obtained by the Washburn (Washburn 1921) or Rideal (Rideal 1922) equation, or by the integration of Eq. 3.4.2.1-3 as

$$L = \left(\frac{\gamma}{2\mu} r \cos\theta \right)^{0.5} t^{0.5} \tag{3.4.2.1-4}$$

There have been many improvements to this equation that take into account tortuosity (crooked or non-straight nature of the capillary channels in the porous medium), wettability of the liquid, and other relevant parameters. As a starting point for further reading, the interested reader is referred to the paper by Yang et al. (1988).

3.4.3 Tangential Annular Flow

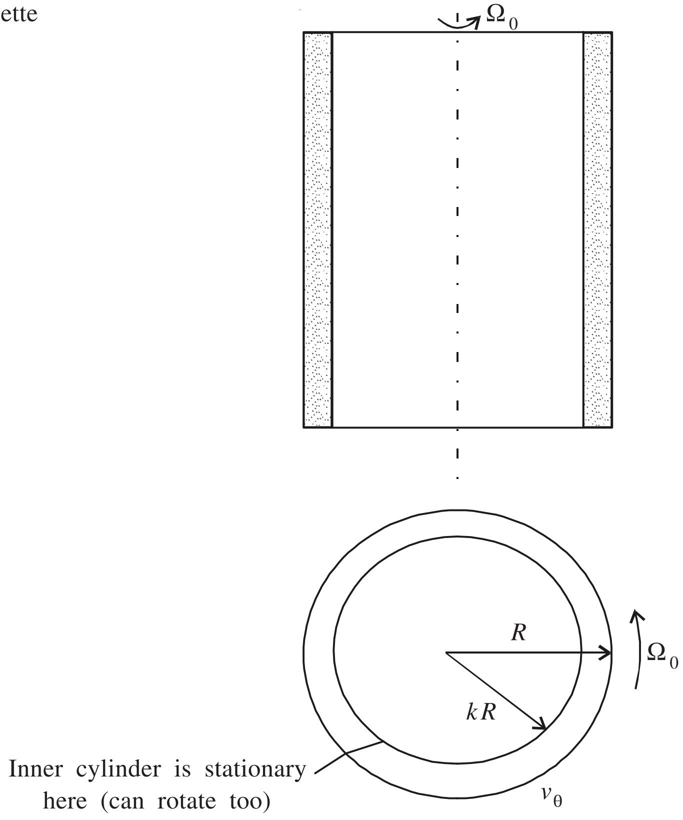
Tangential annular flow between two concentric cylinders is used in couette-flow rheometers to measure viscosity of a variety of biological fluids or bio-products such as xanthan gum. It is also used to study the effects of a 'defined' shear on cells (Sahoo et al. 2003). For our study, let us first consider the tangential annular flow of a Newtonian fluid (Fig. 3.4.3-1). We are interested in the tangential velocity profile between the cylinders, the relevant shear stress distribution, and the torque which is required to turn the outer shaft at steady state.

This is a cylindrical system, and hence it is most convenient to use cylindrical coordinates for analysis. From Eq. A2 of Table 3.4-2, we get the equation of motion in the r direction as

$$\rho\left(\overset{\substack{=0,\ \mathrm{SS}\\ v_r=0}}{\cancel{\frac{\partial v_r}{\partial t}}} + \overset{\substack{=0,\\ v_r=0}}{\cancel{v_r \frac{\partial v_r}{\partial r}}} + \overset{\substack{=0,\\ v_r \neq f(\theta)}}{\cancel{\frac{v_\theta}{r}\frac{\partial v_r}{\partial \theta}}} - \frac{v_\theta^2}{r} + \overset{\substack{=0,\\ v_z=0}}{\cancel{v_z \frac{\partial v_r}{\partial z}}} \right)$$

$$= -\frac{\partial p}{\partial r} + \mu\left(\overset{\substack{=0,\\ v_r=0}}{\cancel{\frac{\partial}{\partial r}\left(\frac{1}{r}\frac{\partial}{\partial r}(r v_r)\right)}} + \overset{\substack{=0,\\ v_r=0}}{\cancel{\frac{1}{r^2}\frac{\partial^2 v_r}{\partial \theta^2}}} - \overset{\substack{=0,\\ v_\theta \neq f(\theta)}}{\cancel{\frac{2}{r^2}\frac{\partial v_\theta}{\partial \theta}}} + \overset{\substack{=0,\\ v_r=0}}{\cancel{\frac{\partial^2 v_r}{\partial z^2}}} \right) + \overset{\substack{=0,\\ g_r=0}}{\cancel{\rho g_r}}$$

Fig. 3.4.3-1 Couette viscometer



Thus

$$-\rho\frac{v_\theta^2}{r}=-\frac{\partial p}{\partial r} \tag{3.4.3-1}$$

From Eq. B2 of Table 3.4-2 (θ component)

$$\rho\left(\overset{=0\ (\mathrm{SS})}{\cancel{\frac{\partial v_\theta}{\partial t}}}+v_r\overset{\substack{(v_r=0)\\0}}{\cancel{\frac{\partial v_\theta}{\partial r}}}+\frac{v_\theta}{r}\overset{\substack{v_\theta\neq f(\theta)\\0}}{\cancel{\frac{\partial v_\theta}{\partial \theta}}}+\overset{\substack{(v_r=0)\\0}}{\cancel{\frac{v_r v_\theta}{r}}}+v_z\overset{\substack{(v_z=0)\\0}}{\cancel{\frac{\partial v_\theta}{\partial z}}}\right)=-\frac{1}{r}\overset{\substack{=0\ (p\text{ not}\\ \text{a }f(\theta))}}{\cancel{\frac{\partial p}{\partial \theta}}}$$

$$+\mu\left[\frac{\partial}{\partial r}\left(\frac{1}{r}\frac{\partial}{\partial r}(r v_\theta)\right)+\frac{1}{r^2}\overset{\substack{v_\theta\neq f(\theta)\\0}}{\cancel{\frac{\partial^2 v_\theta}{\partial \theta^2}}}+\frac{2}{r^2}\overset{\substack{v_r\neq f(\theta)\\0}}{\cancel{\frac{\partial v_r}{\partial \theta}}}+\overset{\substack{v_\theta\neq f(\theta)\\0}}{\cancel{\frac{\partial^2 v_\theta}{\partial z^2}}}\right]+\overset{\substack{(g_\theta=0)\\0}}{\cancel{\rho g_\theta}}$$

In the above equation, $p \neq f(\theta)$ because the points at different angles at the same radial position cannot have different pressures.

Thus

$$0 = \mu\left[\frac{d}{dr}\left(\frac{1}{r}\frac{d}{dr}(rv_\theta)\right)\right] \tag{3.4.3-2}$$

Since r is the only variable, the partial derivatives have been converted into ordinary derivatives.

For the z component

$$\rho\left(\cancelto{= 0\ (\mathrm{SS})}{\frac{\partial v_z}{\partial t}} + v_r \overset{(v_r = 0)}{\cancelto{0}{\frac{\partial v_z}{\partial r}}} + \frac{v_\theta}{r}\overset{v_z \neq f(\theta)}{\cancelto{0}{\frac{\partial v_z}{\partial \theta}}} + v_z \overset{(v_z = 0)}{\cancelto{0}{\frac{\partial v_z}{\partial z}}}\right)$$

$$= -\frac{\partial p}{\partial z} + \mu\left[\frac{1}{r}\frac{\partial}{\partial r}\left(r \overset{(v_z = 0)}{\cancelto{0}{\frac{\partial v_z}{\partial r}}}\right) + \frac{1}{r^2}\overset{(v_z = 0)}{\cancelto{0}{\frac{\partial^2 v_z}{\partial \theta^2}}} + \overset{(v_z = 0)}{\cancelto{0}{\frac{\partial^2 v_z}{\partial z^2}}}\right] + \rho g_z$$

Thus

$$0 = -\frac{\partial p}{\partial z} + \rho g_z \tag{3.4.3-3}$$

Integrating Eq. 3.4.3-3 with the boundary conditions (BCs) given below

At $r = kR$, $v_\theta = 0$ (inner cylinder is stationary)

At $r = R$, $v_\theta = \Omega_0 R$

$$\left[\frac{d}{dr}\left(\frac{1}{r}\frac{d}{dr}(rv_\theta)\right)\right] = 0$$

$$\frac{1}{r}\frac{d}{dr}(rv_\theta) = C_1$$

$$\frac{d}{dr}(rv_\theta) = C_1 r$$

Let $(rv_\theta) = m$

$$\frac{d}{dr}m = C_1 r$$

$$m = \frac{C_1 r^2}{2} + C_2$$

$$rv_\theta = \frac{C_1 r^2}{2} + C_2$$

$$v_\theta = \frac{C_1 r}{2} + \frac{C_2}{r}$$

Using the first BC, we get

$$0 = \frac{C_1}{2}(kR) + \frac{C_2}{kR}$$

$$C_1 = -\left(\frac{C_2}{kR}\right)\times\frac{2}{kR} = -\frac{2C_2}{k^2R^2}$$

Using the second BC, we get

$$\Omega_0 R = -\frac{\cancel{2}C_2}{k^2R^{\cancel{2}}}\times\frac{\cancel{R}}{\cancel{2}} + \frac{C_2}{R}$$

$$\Omega_0 R = C_2\left(\frac{1}{R} - \frac{1}{Rk^2}\right) = \frac{C_2}{R}\left(1 - \frac{1}{k^2}\right) = \frac{C_2}{R}\left(\frac{k^2-1}{k^2}\right)$$

$$C_2 = \frac{\Omega_0 R^2 k^2}{k^2 - 1}$$

$$C_1 = -\frac{2}{k^2R^2}\left(\frac{\Omega_0 R^2 k^2}{k^2-1}\right)$$

$$= -\left(\frac{2\Omega_0}{k^2-1}\right)$$

Therefore

$$v_\theta = -\frac{2\Omega_0}{k^2-1}\cdot\frac{r}{2} + \frac{\Omega_0 k^2 R^2}{(k^2-1)r}$$

$$= \frac{\Omega_0 R^2}{(1-k^2)}\left(\frac{r}{R^2} - \frac{k^2}{r}\right)$$

$$= \frac{\Omega_0 k R^2}{(1-k^2)}\left(\frac{r}{kR^2} - \frac{k}{r}\right)$$

$$= \frac{\Omega_0 R^2}{\frac{1}{k} - k}\,\frac{1}{R}\left(\frac{r}{kR} - \frac{kR}{r}\right)$$

$$v_\theta = \frac{\Omega_0 R\left(\frac{kR}{r} - \frac{r}{kR}\right)}{\left(k - \frac{1}{k}\right)} \tag{3.4.3-4}$$

The relevant shear stress distribution can also be obtained by using the expression for the shear stress components in cylindrical coordinates as given in Table 3.4-5. From Eq. A

$$\tau_{r\theta} = -\mu\left[r\frac{\partial}{\partial r}\left(\frac{v_\theta}{r}\right) + \frac{1}{r}\frac{\partial v_r}{\partial \theta}\right]$$

In this case

$$\tau_{r\theta} = -\mu\left[r\frac{\partial}{\partial r}\left(\frac{v_\theta}{r}\right) + \frac{1}{r}\overset{0(v_r \neq f(\theta))}{\cancel{\frac{\partial v_r}{\partial \theta}}}\right]$$

Using Eq. 3.4.3-4 (since r is the only independent variable, the partial derivatives can be replaced with total derivatives), we get

$$\tau_{r\theta} = -\mu\left[r\frac{d}{dr}\left\{\frac{\Omega_0 R\left(\frac{kR}{r} - \frac{r}{kR}\right)}{r\left(k - \frac{1}{k}\right)}\right\}\right]$$

$$= -\frac{\mu\Omega_0 R}{\left(k - \frac{1}{k}\right)}\left[r\frac{d}{dr}\left(\frac{1}{r}\left\{\frac{kR}{r} - \frac{r}{kR}\right\}\right)\right]$$

$$= -\frac{\mu\Omega_0 R}{\left(k - \frac{1}{k}\right)}\left[r\frac{d}{dr}\left(\frac{kR}{r^2} - \frac{1}{kR}\right)\right]$$

$$= -\frac{\mu\Omega_0 R}{\left(k - \frac{1}{k}\right)}\left[r\left(-\frac{2kR}{r^3}\right)\right]$$

$$= -\frac{2\mu\Omega_0 R^2 k}{\left(k - \frac{1}{k}\right)}\left(\frac{1}{r^2}\right)$$

$$\tau_{r\theta} = -2\mu\Omega_0 R^2\left(\frac{k^2}{k^2 - 1}\right)\left(\frac{1}{r^2}\right) \tag{3.4.3-5}$$

The torque that is needed to turn the outer cylinder

$$= \text{Force} \times \text{Lever arm distance}$$

$$= -\, \tau_{r\theta}\big|_{r=R} \times \text{Area} \times \text{Lever arm distance}$$

(the negative sign before $\tau_{r\theta}$ is to overcome the shear stress by the fluid on the wall)

$$= -\, \tau_{r\theta}\big|_{r=R} \times (2\pi RL) \times R$$

$$= 2\mu\Omega_0 R^2 \left(\frac{k^2}{1-k^2}\right)\left(\frac{1}{R^2}\right) \times 2\pi RL \times R$$

$$= 4\pi\mu\Omega_0 LR^2 \left(\frac{k^2}{1-k^2}\right) \qquad (3.4.3\text{-}6)$$

3.4.4 Dimensionless Numbers and Non-dimensional Analysis

As briefly mentioned in Chapter 2, when certain physical quantities are combined suitably, the resulting quantity or 'number' does not possess any dimensions. For example, as we have seen in Eq. 3.2-1, the quantity, $\frac{\rho v d}{\mu}$ is dimensionless, and is called the Reynolds number.

There are many advantages in using non-dimensional numbers, or in expressing relations in terms of non-dimensional numbers. Such relations may be applied more generally rather than be restricted to a particular, say, tube diameter, as we have already seen in Section 3.2 for the occurrence of, say, laminar flow in tubes. To explain further, it does not matter what the particular values of fluid density, fluid velocity, fluid viscosity and pipe diameter are; as long as their appropriate combination, the Reynolds number, is less than 2100, it will result in laminar flow.

Other advantages in using dimensionless numbers will become evident in the following sections. Since we have brought up the aspect of non-dimensional numbers, let us explore one more powerful possibility of obtaining useful relationships for design and operation, with them. The basis for this powerful possibility is Buckingham's pi theorem.

Buckingham's Pi Theorem

If there are n variables in a problem, and these variables contain m primary dimensions (e.g. M, L, T, and so three for this combination of primary dimensions), the equation relating all the variables will have ($n - m$) dimensionless groups. Buckingham called these dimensionless groups as π groups.

Mathematically, it can be expressed as

$$f(\pi_1, \pi_2, \ldots, \pi_{n-m}) = 0 \tag{3.4.4-1}$$

The π groups must be independent of each other. In other words, it must not be possible to express any π group as some combination of the other π groups.

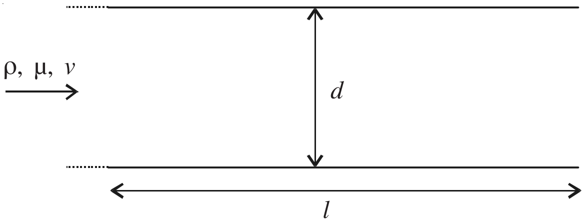
Let us look at dimensions first:

Fundamental	
Mass	[M]
Length	[L]
Time	[T]
Flow Geometry	
Area	[L^2]
Volume	[L^3]
Kinematic	
Velocity	[LT^{-1}]
Acceleration	[LT^{-2}]
Kinematic viscosity	[L^2T^{-1}]
Dynamic	
Force	[MLT^{-2}]
Pressure	[$ML^{-1}T^{-2}$]
Work	[ML^2T^{-2}]
Energy	[ML^2T^{-2}]
Power	[ML^2T^{-3}]
Momentum	[MLT^{-1}]
Density	[ML^{-3}]
Viscosity	[$ML^{-1}T^{-1}$]
Surface tension	[MT^{-2}]

Two conditions need to be satisfied to successfully apply the method to get useful relationships:

1. Each of the fundamental dimensions must appear in at least one of the n variables.

Fig. 3.4.4-1 Flow in a cylindrical pipe



2. It must not be possible to form a dimensionless group by using some of the variables themselves or the variables raised to some powers, within a recurring set. A recurring set is a group of variables that form the dimensionless groups.

Let us apply this method to a situation that we have already seen – to get an expression for pressure drop Δp in a straight pipe (Fig. 3.4.4-1).

Δp is expected to depend on d, l, ρ, μ, v. In other words

$$f(\Delta p, d, l, \rho, \mu, v) = 0$$

The set of variables within the brackets is the recurring set.

Number of variables (n): 6
Number of fundamental dimensions (m): 3 (M, L, T)

Therefore, from the Buckingham pi theorem, the number of dimensionless groups: $n - m = 6 - 3 = 3$.

Also, from experience, it is known that the recurring set must contain 3 (the same number as the number of dimensionless groups) variables that cannot themselves be formed into a dimensionless group. Thus, l and d cannot be chosen together since (l/d) is dimensionless. Δp, ρ and v cannot be chosen together since ($\Delta p/\rho v^2$) is dimensionless. Therefore, let us choose d, v and ρ.

The dimensions are

$$d = [\mathrm{L}]$$
$$v = [\mathrm{LT}^{-1}]$$
$$\rho = [\mathrm{ML}^{-3}]$$

Let us rewrite the dimensions in terms of the chosen variables.

$$[\mathrm{L}] = d$$
$$[\mathrm{M}] = \rho d^3$$
$$[\mathrm{T}] = dv^{-1}$$

Now let us take the remaining variables, Δp, l and μ, in turn. First

$$\Delta p = [\mathrm{ML^{-1}T^{-2}}]$$

Therefore

$$\Delta p[\mathrm{M^{-1}LT^{2}}] \text{ is dimensionless}$$

Thus

$$\begin{aligned}\pi_1 &= \Delta p\ (\rho d^3)^{-1}(d)\ (d^{-1}v)^2\\ &= \Delta p/\rho v^2\end{aligned}$$

Now, let us consider the length, l

$$l = [\mathrm{L}]$$

Therefore

$$l[\mathrm{L}]^{-1} \text{ is dimensionless}$$

Thus

$$\pi_2 = l/d$$

Now, finally, let us consider μ

$$\mu = [\mathrm{ML^{-1}T^{-1}}]$$

Therefore

$$\mu\ [\mathrm{M^{-1}LT}] \text{ is dimensionless}$$

Thus

$$\begin{aligned}\pi_3 &= \mu(\rho d^3)^{-1}(d)\ (dv^{-1})\\ &= \frac{\mu}{\rho v d} \text{ or } 1/N_{\mathrm{Re}}\end{aligned}$$

From the Buckingham's pi theorem

$$\frac{\Delta p}{\rho v^2} = f\left(\frac{1}{d}, \frac{1}{N_{\mathrm{Re}}}\right)$$

or

$$\frac{\Delta p}{\rho v^2} = k\left(\frac{1}{d}\right)^a \left(\frac{1}{N_{\mathrm{Re}}}\right)^b$$

Thus, from a mere dimensional analysis, we know the form of the relationship between the relevant variables. Let us see the validity of what we have got by comparing the above relation to what we already know. We had seen earlier, in pipe flow, the volumetric flow rate

$$Q = \frac{\pi \Delta p}{8\mu l} r^4$$

or

$$Av = \frac{\pi \Delta p}{8\mu l}\left(\frac{d}{2}\right)^4$$

$$(\cancel{\pi} d^2 / 4)v = \frac{\cancel{\pi}\Delta p}{2\cancel{8}\mu l}\left(\frac{d}{2}\right)^4$$

$$\Delta p = (v\cancel{d}^{\cancel{2}}\mu l \times 32)/(d^{\cancel{4}\,2}) = 32\left(\frac{\mu v}{d}\right)\left(\frac{l}{d}\right)$$

$$\frac{\Delta p}{\rho v^2} = 32\left(\frac{\mu}{\rho v d}\right)\left(\frac{l}{d}\right)$$

$$= 32\left(\frac{1}{N_{\mathrm{Re}}}\right)\left(\frac{l}{d}\right)$$

$$\frac{\Delta p}{\rho v^2} = f\left(\frac{1}{N_{\mathrm{Re}}}, \frac{l}{d}\right) \text{and } a = b = 1; k = 32$$

3.5 Unsteady State Flow

Let us consider a fluid that is initially at rest in a circular tube. At $t = 0$, the fluid is set in motion by an axial pressure gradient, say $\frac{\Delta p}{L}$ where Δp is the difference in pressure (pressure drop) across the tube of length L. From the time the pressure gradient is applied to the time the steady state is achieved, the velocity profile across the cross-section of the tube at, say a certain location on the length of the tube varies. At that location, let us study the time-dependant (unsteady state) variation of velocity profiles. Also, note that we have implicitly assumed that at any time in the tube the flow will be in cylindrical layers (laminar).

Let us first take Eq. C2 of Table 3.4-2 (the z component of the equation of motion in cylindrical coordinates), and simplify it by cancelling the irrelevant terms.

$$\rho\left(\frac{\partial v_z}{\partial t} + v_r \cancelto{v_r = 0}{\frac{\partial v_z}{\partial r}} + \frac{v_\theta}{r} \cancelto{v_\theta = 0}{\frac{\partial v_z}{\partial \theta}} + v_z \frac{\partial v_z}{\partial z}\right)$$

$$= -\frac{\partial p}{\partial z} + \mu\left(\frac{1}{r}\frac{\partial}{\partial r}\left(r\frac{\partial v_z}{\partial r}\right) + \frac{1}{r^2}\cancelto{v_z \neq f(\theta)}{\frac{\partial^2 v_z}{\partial \theta^2}} + \frac{\partial^2 v_z}{\partial z^2}\right) + \rho g_z$$

$$\rho\frac{\partial v_z}{\partial t} + v_z\frac{\partial v_z}{\partial z} = -\frac{\partial(p - \rho g z)}{\partial z} + \frac{\mu}{r}\frac{\partial}{\partial r}\left(r\frac{\partial v_z}{\partial r}\right) + \mu\frac{\partial^2 v_z}{\partial z^2}$$

The above equation is very complex to solve. To be able to get some insights, let us make it amenable to an analytical solution, however tedious – this can be done by making an approximation, $v_z \neq f(z)$. In other words, it is assumed that at a particular time, the axial velocity at a particular radial position does not vary with the length of the tube – this may not be a bad assumption. Making suitable assumptions and approximations are essential in engineering practice, and is mostly an art. Thus, the equation to solve becomes

$$\rho\frac{\partial v_z}{\partial t} = -\frac{\partial(p - \rho g z)}{\partial z} + \frac{\mu}{r}\frac{\partial}{\partial r}\left(r\frac{\partial v_z}{\partial r}\right) \qquad (3.5\text{-}1)$$

with

IC: At $t = 0$, $v_z = 0$

BC 1: At $r = 0$, $v_z =$ finite or $\dfrac{\partial v_z}{\partial z} = 0$

BC 2: At $r = R$, $v_z = 0$

Since p does not vary with time once the flow begins or with r (as seen earlier, and which is also valid here), $p - \rho g z = P = f(z)$ alone. Thus, the partial derivative $\dfrac{\partial P}{\partial z}$ can be replaced with the total derivative, $\dfrac{dP}{dz}$.

Therefore

$$\frac{dP}{dz} = \text{Constant} = \frac{\Delta P}{L}$$

where

$$\Delta P = P_L - P_0$$

Thus, Eq. 3.5-1 can be written as

$$\rho\frac{\partial v_z}{\partial t}=-\frac{\Delta P}{L}+\frac{\mu}{r}\frac{\partial}{\partial r}\left(r\frac{\partial v_z}{\partial r}\right) \tag{3.5-2}$$

Use of dimensionless variables usually simplifies analysis. Let us define the following dimensionless variables.

$$\phi=\frac{v_z}{(-\Delta P)R^2/4\mu L}=\frac{v_z}{v_{z,\max}} \tag{3.5-3}$$

$$\xi = r/R \tag{3.5-4}$$

$$\tau=\frac{\nu t}{R^2} \tag{3.5-5}$$

where $\nu=\frac{\mu}{\rho}$, the kinematic viscosity.

From the above definitions

$$v_z=\frac{(-\Delta P)R^2}{4\mu L}\phi$$

$$r = \xi R$$

$$t=\frac{R^2\tau}{\nu}$$

Thus

$$\frac{\partial v_z}{\partial t}=\frac{(-\Delta P)\cancel{R^2}}{4\mu L}\times\frac{\nu}{\cancel{R^2}}\frac{\partial\phi}{\partial\tau}$$

$$\rho\frac{\partial v_z}{\partial t}=\frac{\cancel{\rho}(-\Delta P)\times\cancel{\mu}}{4\cancel{\mu}L\cancel{\rho}}\frac{\partial\phi}{\partial\tau}=\frac{(-\Delta P)}{4L}\frac{\partial\phi}{\partial\tau}$$

Further

$$r\frac{\partial v_z}{\partial r}=\xi R\frac{\partial\left(\frac{(-\Delta P)R^2}{4\mu L}\phi\right)}{\partial(\xi R)}=\frac{\left(\xi R\frac{(-\Delta P)R^2}{4\mu L}\partial\phi\right)}{R\quad\partial(\xi)}=\frac{\xi(-\Delta P)R^2}{4\mu L}\frac{\partial\phi}{\partial\xi}$$

$$\frac{\mu}{r}\frac{\partial}{\partial r}\left(r\frac{\partial v_z}{\partial r}\right)=\frac{\mu}{R\xi}\frac{\partial}{\partial(R\xi)}\left(\frac{\xi(-\Delta P)R^2}{4\mu L}\frac{\partial\phi}{\partial\xi}\right)$$

$$=\frac{\mu}{R^2}\frac{1}{\xi}\frac{(-\Delta P)R^2}{4\mu L}\frac{\partial}{\partial\xi}\left(\xi\frac{\partial\phi}{\partial\xi}\right)$$

$$=\frac{(-\Delta P)}{4L}\frac{1}{\xi}\frac{\partial}{\partial\xi}\left(\xi\frac{\partial\phi}{\partial\xi}\right)$$

Through substitution of the above expressions in Eq. 3.5-2 we get

$$\frac{(-\Delta P)}{4L}\frac{\partial\phi}{\partial\tau}=\frac{(-\Delta P)}{L}+\frac{(-\Delta P)}{4L}\frac{1}{\xi}\frac{\partial}{\partial\xi}\left(\xi\frac{\partial\phi}{\partial\xi}\right)$$

$$\frac{\partial\phi}{\partial\tau}=4+\frac{1}{\xi}\frac{\partial}{\partial\xi}\left(\xi\frac{\partial\phi}{\partial\xi}\right) \tag{3.5-6}$$

IC: At $\tau = 0$, $\phi = 0$

BC 1: At $\xi = 0$, ϕ = finite, or $\dfrac{\partial\phi}{\partial\xi} = 0$

BC 2: At $\xi = 1$, $\phi = 0$

For a steady state flow, we can use Eq. 3.4.2-15 to get

$$v_z=\frac{(-\Delta P)R^2}{4\mu L}\left\{1-\left(\frac{r}{R}\right)^2\right\}$$

We can write the relationship in terms of dimensionless variables as

$$\phi_\infty = 1 - \xi^2 \tag{3.5-7}$$

where $\phi_\infty = \phi(\tau = \infty)$ i.e. when steady state is reached.

ϕ can be written in terms of a 'steady state' value and a 'deviation' value i.e.

$$\phi(\xi, \tau) = \phi_\infty(\xi) - \phi_t(\xi, \tau) \tag{3.5-8}$$

where $\phi_t(\xi, \tau)$ is the deviation value that represents the 'deviation from steady state'. Thus

$$\frac{\partial\phi}{\partial\tau}=\frac{\partial(\phi_\infty-\phi_t)}{\partial\tau}$$

$$=-\frac{\partial\phi_t}{\partial\tau} \quad \because \phi_\infty \neq f(\tau)$$

Also

$$\frac{1}{\xi}\frac{\partial}{\partial\xi}\left(\xi\frac{\partial\phi}{\partial\xi}\right)=\frac{1}{\xi}\frac{\partial}{\partial\xi}\left(\xi\frac{\partial(\phi_\infty-\phi_t)}{\partial\xi}\right)$$

$$=\frac{1}{\xi}\frac{\partial}{\partial\xi}\left(\xi\frac{\partial(1-\xi^2-\phi_t)}{\partial\xi}\right)$$

$$=\frac{1}{\xi}\frac{\partial}{\partial\xi}\left(\xi\left\{-2\xi-\frac{\partial\phi_t}{\partial\xi}\right\}\right)$$

$$= \frac{1}{\xi}\frac{\partial}{\partial \xi}\left((-2\xi^2) - \xi\frac{\partial \phi_t}{\partial \xi} \right)$$

$$= \frac{1}{\xi}\left[-4\xi - \frac{\partial}{\partial \xi}\left(\xi\frac{\partial \phi_t}{\partial \xi} \right) \right]$$

$$= -4 - \frac{1}{\xi}\frac{\partial}{\partial \xi}\left(\xi\frac{\partial \phi_t}{\partial \xi} \right)$$

Substituting the above in Eq. 3.5-6, we get

$$-\frac{\partial \phi_t}{\partial \tau} = 4 - 4 - \frac{1}{\xi}\frac{\partial}{\partial \xi}\left(\xi\frac{\partial \phi_t}{\partial \xi} \right)$$

$$\frac{\partial \phi_t}{\partial \tau} = \frac{1}{\xi}\frac{\partial}{\partial \xi}\left(\xi\frac{\partial \phi_t}{\partial \xi} \right) \tag{3.5-9}$$

Now, the initial and boundary conditions are

IC: At $\tau = 0$, $\phi_t = \phi_\infty$ (by substituting $\phi = 0$ in Eq. 3.5-8)
BC 1: At $\xi = 0$, ϕ = finite i.e. (since $\phi_\infty = 0$ from Eq. 3.5-7 and $\phi = 0$ when $\xi = 1$)
BC 2: At $\xi = 1$, $\phi_t = 0$

If we assume that $\phi_t(\xi, \tau)$ is separable as

$$\phi_t(\xi, \tau) = f(\xi) . g(\tau)$$

then

$$\frac{\partial \phi_t}{\partial \tau} = f\frac{dg}{d\tau} \quad \text{and} \quad \frac{\partial \phi_t}{\partial \xi} = g \times \frac{df}{d\xi}$$

Therefore

$$f\frac{dg}{d\tau} = \frac{1}{\xi}\frac{d}{d\xi}\left(\xi g\frac{df}{d\xi} \right)$$

$$f\frac{dg}{d\tau} = g\frac{1}{\xi}\frac{d}{d\xi}\left(\xi\frac{df}{d\xi} \right)$$

$$\frac{1}{g}\frac{dg}{d\tau} = \frac{1}{f}\frac{1}{\xi}\frac{d}{d\xi}\left(\xi\frac{df}{d\xi} \right) \tag{3.5-10}$$

Since the LHS is a function of τ alone and the RHS is a function of ξ alone, for Eq. 3.5-10 to hold at all times, each side must be equal to a constant, say $-k^2$ (negative); the reason for a negative value will be apparent shortly.

$$\frac{1}{g}\frac{dg}{d\tau} = -k^2 \tag{3.5-11}$$

This implies

$$g = C_1 \exp(-k^2\tau) \tag{3.5-12}$$

If $(-k^2)$ is not negative, then g, and consequently ϕ_t cannot diminish to zero at steady state ($\tau = \infty$); thus the constant $(-k^2)$ needs to be negative.

Equation 3.5-10 can be written as

$$\frac{1}{\xi}\frac{d}{d\xi}\left(\xi\frac{df}{d\xi}\right) + k^2 f = 0 \tag{3.5-13}$$

The boundary conditions are given below

BC 1: At $\xi = 0$, f = finite, i.e. $\dfrac{df}{d\xi} = 0$

BC 2: At $\xi = 1$, $f = 0$ (since $\phi_t = 0$ for all g, note that $g = g(\tau)$)

The solution for Eq. 3.5-13 requires knowledge of Bessel functions and their relationships. The student is directed to other appropriate books (e.g. Lih 1974) for a better understanding of the same. Here, we merely present the solution.

The solution is of the form

$$f = c_2 J_0(k\xi) + c_3 Y_0(k\xi) \tag{3.5-14}$$

where J_0 is a Bessel function of the I kind

$$J_0(k\xi) = \sum_{k=0}^{\alpha} \frac{(-1)^r \left(\frac{k\xi}{2}\right)^{2r}}{(r!)^2}$$

Y_0 is a Weber's Bessel function of the II kind

$$Y_0(k\xi) = \frac{2}{\pi}\left[\bar{Y}_0(k\xi) - (\ln 2 - \Gamma) J_0(k\xi)\right]$$

where $\Gamma = \lim_{n\to\infty}\left(1 + \frac{1}{2} + \frac{1}{3} + \ldots + \frac{1}{n} - \ln n\right) = 0.57721\ldots$ (Euler's constant),

and $\bar{Y}_0$ is a Neumann's Bessel function of the II kind.

$$\bar{Y}_0(k\xi) = J_0(k\xi)\int \frac{d\xi}{\xi[J_0(k\xi)]^2}$$

$C_3 = 0$ (from BC 1; otherwise the term would not be finite since $Y_0(0) = -\infty$)

$C_2\, J_0\,(k) = 0$ (from BC 2).

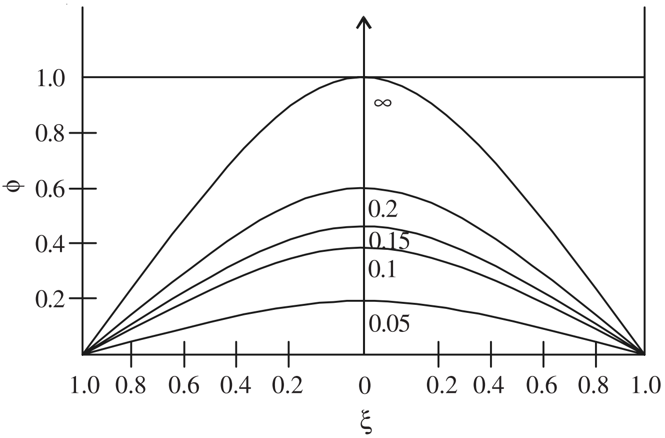


Fig. 3.5-1 Profiles of ϕ at a particular length position on the tube, versus ξ for various values of τ

Now, C_2 cannot be zero since that would result in a trivial solution, ($f = 0$). Therefore

$$J_0\,(k) = 0$$

This happens multiple times when $k = 2.4048...$ ($= k_1$), 5.52009 ($= k_2$), $8.6537...$ ($= k_3$), and so on.

Thus, there are infinite solutions

$$f_n = C_{2n}\, J_0\,(k_n\xi)\ n = 1, 2, 3, \ldots \infty$$

This implies that

$$\phi_{tn} = C'_n J_0(k_n\xi)\ \exp\,(-\,k_n^2\ \tau),\ n = 1, 2, 3, \ldots \infty$$

where $C'_n = C_1 C_{2n}$.

Using the principles of superimposition, orthogonality relationships, and other relevant aspects of Bessel functions, the final solution is

$$\phi(\xi,\tau) = (1-\xi^2) - 8\sum\nolimits_{n=1}^{\infty} \frac{J_0(k_n\xi)}{k_n^3 J_1(k_n)} \exp(-\,k_n^2\tau) \tag{3.5-15}$$

A representative plot of ϕ versus ξ for various values of τ is given in Fig. 3.5-1.

3.6 Pulsatile Flow

In the earlier cases, we had considered a linear, time invariant pressure gradient. However, flows in the body, e.g. blood flow through the vasculature are pulsatile in nature because of the pumping of the heart. In other words, the pressure gradient varies with time.

Let us consider here a sinusoidal pressure gradient. Although not strictly valid for blood flow, a time-varying sinusoidal pressure gradient does provide valuable insights into the nature of pulsatile biological flows. Also, let us assume that the axial velocity at a particular radial position does not change with the length of the tube at any given time.

From Eq. C2 of Table 3.4-2 (the z component of the equation of motion)

$$\rho\left(\frac{\partial v_z}{\partial t}+v_r\overset{(v_r=0)}{\cancelto{0}{\frac{\partial v_z}{\partial r}}}+\frac{v_\theta}{r}\overset{(v_\theta=0)}{\cancelto{0}{\frac{\partial v_z}{\partial \theta}}}+v_z\overset{(v_z\neq f(z))}{\cancelto{0}{\frac{\partial v_z}{\partial z}}}\right)$$

$$=-\frac{\partial p}{\partial z}+\mu\left[\frac{1}{r}\frac{\partial}{\partial r}\left(r\frac{\partial v_z}{\partial r}\right)+\frac{1}{r^2}\overset{v_z\neq f(\theta)}{\cancelto{0}{\frac{\partial^2 v_z}{\partial \theta^2}}}+\overset{(v_z\neq f(z))}{\cancelto{0}{\frac{\partial^2 v_z}{\partial z^2}}}\right]+\rho g_z$$

Note that we have taken $v_z \neq f(z)$ at a particular time. Thus, the remaining terms yield

$$\rho\frac{\partial v_z}{\partial t}=-\frac{\partial(p-\rho g z)}{\partial z}+\frac{\mu}{r}\frac{\partial}{\partial r}\left(r\frac{\partial v_z}{\partial r}\right) \tag{3.6-1}$$

By the same arguments as in Section 3.5 that led to Eq. 3.5-2, we can write

$$\frac{\partial P}{\partial z}=\frac{-\Delta P}{L}+A\sin\omega t \tag{3.6-2}$$

where $\frac{-\Delta P}{L}$ is the average pressure gradient; A and ω are the frequency and amplitude, respectively, of the periodic pressure function.

Since $\frac{\mu}{\rho}=\nu$, the equation of motion can be written as

$$\frac{1}{\nu}\frac{\partial v_z}{\partial t}=\frac{1}{r}\frac{\partial}{\partial r}\left(r\frac{\partial v_z}{\partial r}\right)+\frac{(-\Delta P)}{\mu L}+\frac{A}{\mu}\sin\omega t \tag{3.6-3}$$

We can guess that the solution for v_z consists of a steady state part (average value) and a periodic part (fluctuating value) corresponding to the average and fluctuating pressure gradients, i.e.

$$v_z\,(r,\,t)=\bar{v}_z(r)+v_z'\,(r,\,t) \tag{3.6-4}$$

Substituting Eq. 3.6-4 in Eq. 3.6-3, and using separation of variables as in the Section 3.5 with the recognition that $\bar{v}_z(r)$ is not a function of t, gives two equations

$$0 = \frac{1}{r}\left(\frac{d}{dr} r \frac{d\bar{v}_z}{dr}\right) + \frac{(-\Delta P)}{\mu L} \tag{3.6-5}$$

$$\frac{1}{\nu}\frac{\partial v'_z}{\partial t} = \frac{1}{r}\frac{\partial}{\partial r} r \frac{\partial v'_z}{\partial r} + \frac{A}{\mu}\sin \omega t \tag{3.6-6}$$

The solution of Eq. 3.6-5, as seen in an earlier section is

$$\bar{v}_z = \frac{(-\Delta P)R^2}{4\mu L}\left\{1 - \left(\frac{r}{R}\right)^2\right\} \tag{3.6-7}$$

Equation 3.6-6 can be solved by Laplace transforms through a lengthy procedure, with the boundary conditions as

$$\text{BC 1: At } r = 0,\ \frac{\partial \overline{v'_z}}{\partial r} = 0$$

$$\text{BC 2: At } r = R,\ \overline{v'_z} = 0$$

to yield the following as the other part of the solution – the first part being the parabolic profile given by Eq. 3.6-7. Here we merely state the combined solution as follows

$$\begin{aligned} v_z(r,t) &= \frac{(-\Delta P)R^2}{4\mu L}\left\{1 - \left(\frac{r}{R}\right)^2\right\} \\ &+ \frac{2A}{\rho}\sum_{k=1}^{\infty}\frac{J_0\left(\frac{\alpha_k r}{R}\right)}{\alpha_k J_1(\alpha_k)}\left\{\frac{\omega \exp(-\alpha_k^2 \nu t / R^2)}{\left(\frac{\alpha_k^4 \nu^2}{R^4}\right) + \omega^2} + \frac{\sin(\omega t - \phi)}{\sqrt{\left(\frac{\alpha_k^4 \nu^2}{R^4}\right) + \omega^2}}\right\} \end{aligned} \tag{3.6-8}$$

Thus, the velocity profile at a cross-section varies with time from the basal parabolic profile. The variation is cyclic, as can be expected from a cyclic pressure gradient.

3.7 Solutions to Equations

As was evident in the Sections 3.5 and 3.6, the mathematical effort to solve the formulated equations could be significant. An analytical solution is reasonably complete, and capable of rendering itself to confident interpretations due to the continuous nature of this approach. However, an analytical solution may not be available for all situations. Thus, in many research problems, it is common to take a numerical approach, such as the finite element method, to solve the formulated equations. Some level of expertise is needed for the appropriate use and interpretation of numerical solutions. Even if one does not possess such expertise, one can team up with a suitable expert for the solution.

In this section, let us see some formulations for simplifying the solutions of the differential equations. Two of the common approaches are merely mentioned in this section. The reader is referred to other texts (Bird et al. 2002) for the details on these approaches.

3.7.1 Stream Function Approach

Velocity is expressed as the gradient of a 'stream function' say, ψ. For example

$$v_x = -\frac{\partial \psi}{\partial y}$$

$$v_y = +\frac{\partial \psi}{\partial x}$$

ψ = constant (mathematical representation) indicates streamlines (physical significance) i.e. the path traced by the particles of fluid under steady flow.

3.7.2 Boundary Layer Theory

The flow is split into two parts:

- Potential flow (away from the wall) (ρ = constant; $\mu = 0$; flow is irrotational ($\vec{\nabla} \times \vec{v} = 0$))
- Boundary layer flow (close to the wall)

3.8 Turbulent Flow

As seen in Section 3.2, above a certain Reynolds number that is dependent on the system (4000 for pipe flow), the flow turns chaotic or turbulent.

Many flows in the bio-industry occur in the turbulent regime. Turbulent flow can also occur near artificial valves of the heart, which may result in wasteful expenditure of pumping energy.

By careful measurements, it has been experimentally shown that for turbulent flow *in a pipe*, the time-smoothed components (average quantities at a point), $\bar{v}_z$ and $\bar{v}_{z,\text{avg}}$ (these terms will become clearer soon) are related as

---

Turbulent flow Laminar flow

$$\frac{\bar{v}_z}{\bar{v}_{z,\max}} \cong \left(1-\frac{r}{R}\right)^{\frac{1}{7}} \quad = \quad \left[1-\left(\frac{r}{R}\right)^2\right] \tag{3.8-1}$$

$$\frac{\bar{v}_{z,\text{avg}}}{\bar{v}_{z,\max}} \cong \frac{4}{5} \quad = \quad \frac{1}{2} \tag{3.8-2}$$

$$\Delta P \propto Q^{\frac{7}{4}} \quad \propto \quad Q \tag{3.8-3}$$

Turbulent flow can be visualised as the random motion of packets of fluid (eddies). For turbulent flow in a tube, the flow is entirely random at the centre of the tube, i.e. far away from the wall. Near the wall, the fluctuations of velocity in the axial direction is greater than the fluctuations in the radial direction. At the wall, the fluctuations are zero.

Let us take a closer look at these fluctuations. We will focus our attention on the fluid behaviour at one point in the tube (pipe) where turbulent flow exists. As we are watching it, let us say that the mean velocity decreases (probably due to a change in the pressure drop causing the flow, by turning down the pump speed).

The variation of the axial component of the velocity, v_z, at the point of observation, would look like that given in Fig. 3.8-1.

$\bar{v}_z$ is called the time-smoothed velocity, i.e. the average of v_z over a time interval large enough with respect to the time of turbulent oscillation, but small enough with respect to the time changes in the pressure drop causing the flow.

$$\bar{v}_z = \frac{1}{t_a}\int_t^{t+t_a} v_z dt \tag{3.8-4}$$

Thus

$$v_z = \bar{v}_z + v_z' \text{ (average + fluctuation)} \tag{3.8-5}$$

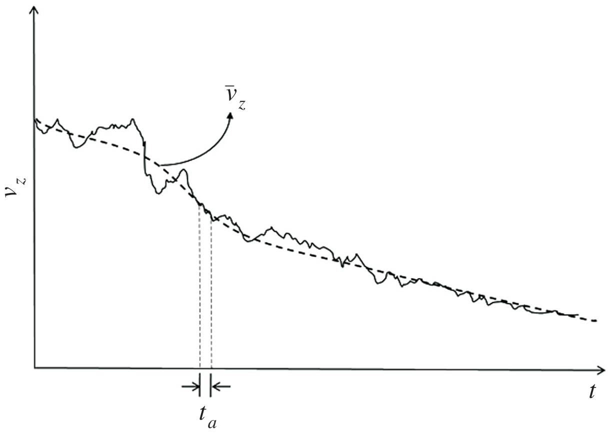


Fig. 3.8-1 Velocity (v_z) and time-smoothed velocity ($\bar{v}_z$) at a point in turbulent flow

The pressure at a point will also vary in a similar fashion

$$p = \bar{p} + p' \tag{3.8-6}$$

If we take the average of the fluctuations, $\bar{v}_z$, since the positive values will balance the negative values

$$\bar{v}'_z = 0 \tag{3.8-7}$$

Thus, we cannot use $\bar{v}'_z$ as a measure of turbulence. However, the average of the squares of the fluctuation values, $\overline{v_z'^2}$, will not be zero and can be used as a measure of turbulence. In fact

$$\text{Intensity of turbulence} \equiv \frac{\sqrt{\overline{v_z'^2}}}{\bar{v}_{z,\text{avg}}} \tag{3.8-8}$$

The intensity of turbulence is typically between 0.01 and 0.1.

At the wall, since the fluctuations in the radial component will be different from those in the axial direction, we need to differentiate between the two. Researchers have found that near the wall

$$\text{(Axial)}\ \frac{\sqrt{\overline{v_z'^2}}}{\bar{v}_{z,\text{avg}}} > \frac{\sqrt{\overline{v_r'^2}}}{\bar{v}_{z,\text{avg}}}\ \text{(Radial)}$$

At the centre of the tube the above values are comparable (isotropic condition).

As long as the eddy size is greater than the mean free path of the molecules (continuum holds), the

- equation of continuity (mass balance)
- equation of motion (momentum balance)

are applicable for turbulent flow. Let us consider the conservation equations for turbulent flow, at a point and take the case for which we have an intuitive feel, i.e. the equation in rectangular Cartesian coordinates. For illustration, let us consider an incompressible flow.

Equation of Continuity

$$\frac{\partial}{\partial x}(\bar{v}_x + v_x') + \frac{\partial}{\partial y}(\bar{v}_y + v_y') + \frac{\partial}{\partial z}(\bar{v}_z + v_z') = 0 \tag{3.8-9}$$

Equation of Motion

x direction

$$\frac{\partial}{\partial t}\rho(\bar{v}_x + v_x') = -\frac{\partial}{\partial x}(\bar{p} + p') - \left[\frac{\partial}{\partial x}\rho(\bar{v}_x + v_x')(\bar{v}_x + v_x') + \frac{\partial}{\partial y}\rho(\bar{v}_y + v_y')(\bar{v}_x + v_x') + \frac{\partial}{\partial z}\rho(\bar{v}_z + v_z')(\bar{v}_x + v_x')\right] + \mu\nabla^2(\bar{v}_x + v_x') + \rho g_x \tag{3.8-10}$$

Taking the time average of the velocity components, i.e. $\bar{v} = \frac{1}{t_a}\int_0^{t_a} v\,dt$ over t_as that are large with respect to turbulent oscillations but small with respect to macro variations, the time-smoothed equation of continuity can be written as follows (note that the time averaged fluctuations will tend to zero)

$$\frac{\partial \bar{v}_x}{\partial x} + \frac{\partial \bar{v}_y}{\partial y} + \frac{\partial \bar{v}_z}{\partial z} = 0 \tag{3.8-11}$$

Similarly, the time-smoothed equation of motion can be written as

$$\frac{\partial}{\partial t}\rho\bar{v}_x = -\frac{\partial \bar{p}}{\partial x} - \left[\frac{\partial}{\partial x}\rho\bar{v}_x\bar{v}_x + \frac{\partial}{\partial y}\rho\bar{v}_y\bar{v}_x + \frac{\partial}{\partial z}\rho\bar{v}_z\bar{v}_x\right] - \left[\frac{\partial}{\partial x}\rho\overline{v_x'v_x'} + \frac{\partial}{\partial y}\rho\overline{v_y'v_x'} + \frac{\partial}{\partial z}\rho\overline{v_z'v_x'}\right] + \mu\nabla^2\bar{v}_x + \rho g_x \tag{3.8-12}$$

The third term in brackets on the RHS of Eq. 3.8-12 is the only extra term when compared to the equation of continuity for laminar flow.

Now, since $\rho\vec{v}\vec{v}$ = momentum flux or stress, let us say that

$$\bar{\tau}_{xx}^{(t)} = \rho\overline{v'_x v'_x}$$

$$\bar{\tau}_{xy}^{(t)} = \rho\overline{v'_x v'_y}$$

and so on.

These are the components of the turbulent momentum flux tensor $\bar{\tilde{\tau}}^{(t)}$. The stresses are also known as Reynolds stresses.

In vector notation, the time-smoothed equation of continuity is

$$\vec{\nabla}.\bar{\vec{v}} = 0 \tag{3.8-13}$$

and the time-smoothed equation of motion is

$$\rho\frac{D\bar{\vec{v}}}{Dt} = -\vec{\nabla}\,\bar{p} - \left[\vec{\nabla}.\bar{\tilde{\tau}}^{(l)}\right] - \left[\vec{\nabla}.\bar{\tilde{\tau}}^{(t)}\right] + \rho\vec{g} \tag{3.8-14}$$

The above Eqs. (3.8-9) to (3.8-14) are valid for an incompressible flow. Similarly, it can be shown that the earlier equations and the tables for laminar flow are valid if we replace

v_i by $\bar{v}_i$

p by $\bar{p}$

and τ_{ij} by $\bar{\tau}_{ij}^{(l)} + \bar{\tau}_{ij}^{(t)}$

However, to get the velocity profile, we need a relationship between τ and the velocity gradient.

For laminar flow, we had a theoretical base in terms of constitutive equations. For turbulent flow, we do not have that luxury. Nevertheless, many expressions based on experimental observations have been proposed. Two are given below.

The first is on the same lines as for the laminar case.

$$\bar{\tau}_{yx}^{(t)} = -\,\mu^{(t)}\frac{d\,\bar{v}_x}{dy} \tag{3.8-15}$$

where $\mu^{(t)}$ is termed as ‘eddy viscosity’ and its value could be hundreds of times the molecular viscosity.

Another popular expression was formulated by Prandtl. For this expression, it is assumed that the eddies in the fluid move around in a fashion similar to that of the molecules in a gas. A ‘mixing length’, l, which is a function of position represents an idea similar to the ‘mean free path’ in the kinetic theory of gases. The relationship is given as

$$\bar{\tau}_{yx}^{(t)} = -\rho l^2 \left|\frac{d\bar{v}_x}{dy}\right| \frac{d\bar{v}_x}{dy} \tag{3.8-16}$$

For flow in pipes/tubes, the relationship between velocity and distance (velocity profile) in turbulent flow through Deissler's empirical formulation is as follows:

If we define

$$v^+ = \frac{\bar{v}_z}{\sqrt{\frac{\tau_0}{\rho}}}$$

and

$$s^+ = s\left(\sqrt{\frac{\tau_0}{\rho}}\right)\frac{\rho}{\mu}$$

where $s = R - r$ i.e. the radial distance from the wall and τ_0 is wall shear stress at $s = 0$.

For $s^+ > 26$

$$v^+ = \frac{1}{0.36}\ln s^+ + 3.8 \tag{3.8-17}$$

For $0 \le s^+ \le 5$

$$v^+ = s^+ \tag{3.8-18}$$

And for $0 \le s^+ \le 26$

$$v^+ = \int_0^{s^+} \frac{ds^+}{1 + n^2 v^+ s^+ (1 - \exp\{-n^2 v^+ s^+\})} \tag{3.8-19}$$

where n is Deissler's constant for tube flow, near the wall. It was found empirically to be equal to 0.124.

3.9 Macroscopic Aspects: The Engineering Bernoulli Equation

Although the understanding of fluid flow thus far was in good depth, the mathematical effort was significant. If we can reduce the effort, but still get acceptable answers, it may be good for engineering design and operation. The 'engineering Bernoulli equation' is useful for this purpose.

To arrive at the engineering Bernoulli equation, one can begin with the equation of motion, Eq. 3.4-4. The details of the lengthy and mathematically involved derivation are indicated in different sections of Bird et al. (2002). Some details are highlighted here.

First, the dot product of the velocity vector, $\vec{v}$, is taken with the equation of motion, i.e. Eq. 3.4-4. Then, skilful rearrangement of terms, the application of the equation of continuity, and representation of the acceleration due to gravity term as the negative gradient of a scalar potential per unit mass (we will do operations similar to some of the above, later in Chapter 4), followed by further rearrangement of terms, leads to an equation of mechanical energy (the kinetic energy alone, the potential energy alone, and the sum of kinetic and potential energies are examples of 'mechanical energy'), which is given below as Eq. 3.9-1. Please note that the mechanical energy is not conserved.

$$\frac{\partial\left(\frac{1}{2}\rho v^2+\rho\phi\right)}{\partial t}=-\left(\vec{\nabla}\cdot\left(\frac{1}{2}\rho v^2+\rho\phi\right)\vec{v}\right)-(\vec{\nabla}\cdot p\vec{v})-p(-\vec{\nabla}\cdot\vec{v})-(\vec{\nabla}\cdot(\tilde{\tau}\cdot\vec{v}))-(-\tilde{\tau}:\vec{\nabla}\vec{v}) \tag{3.9-1}$$

Equation 3.9-1 is a differential equation, which can be integrated over the volume of the macroscopic system of interest. The integration procedure needs the knowledge of the three-dimensional Leibniz formula, Gauss divergence theorem, etc. After further rearrangement of terms, the integrated equation can be written as

$$\frac{d\left(\int_V\left(\frac{1}{2}\rho v^2+\rho\phi\right)\right)}{dt}=-\Delta\left[\dot{m}\left(\frac{p}{\rho}+\frac{1}{2}v^2+gz\right)\right]+\int_V p(\vec{\nabla}\cdot\vec{v})dV+\int_V(\tilde{\tau}:\vec{\nabla}\vec{v})dV-(-W_s) \tag{3.9-2}$$

where the Δ represents the difference in the relevant variables between the two positions, say the ends of the volume of interest e.g. entry and exit points of a pipe through which a fluid is flowing. W_s refers to the work done on the fluid, say by a pump, and is the negative of the work done by the system/control volume on the fluid. Also note that the LHS is the time derivative of the sum of kinetic and potential energies that is obtained by integrating Eq. 3.9-1 over the relevant volume.

The term $\int_V p(\vec{\nabla}\cdot\vec{v})dV$ denotes compression or expansion experienced by the fluid in the relevant volume of interest. It is zero for incompressible fluids.

The term $\int_V(\tilde{\tau}:\vec{\nabla}\vec{v})dV$ represents what can be simplistically said to be energy loss due to viscous effects, or viscous dissipation. For Newtonian fluids, this term is negative, and thus, represents a loss. However, the same cannot be generalised to all fluids.

Now, at steady state, the LHS of Eq. 3.9-2 is zero. Further, under the assumption of a 'representative streamline' through the system, and for a constant mass flow rate $(\dot{m})$ between the two positions of interest (say 1 and 2), the following combination of terms can be approximately made:

$$\dot{m}\Delta\left(\frac{p}{\rho}\right) - \int_V p(\vec{\nabla}\cdot\vec{v})\,dV \approx \dot{m}\int_1^2 \frac{1}{\rho}\,dp \tag{3.9-3}$$

Further, with the assumption that

$$\frac{(v^3)_{\text{avg}}}{v_{\text{avg}}} \approx v_{\text{avg}}^2 \text{ or say, } v^2 \tag{3.9-4}$$

and by division throughout by $\dot{m}$, we can write Eq. 3.9-2, under all the above assumptions, including that of an incompressible fluid as

$$\frac{\Delta p}{\rho} + \frac{\Delta v^2}{2} + g\Delta x + \widehat{FL} + \widehat{W_s} = 0 \tag{3.9-5}$$

where

$$\widehat{FL} = -\frac{1}{\dot{m}}\int (\tilde{\tau} : \vec{\nabla}\vec{v})\,dV$$

$$\widehat{W_s} = \frac{1}{\dot{m}} W_s$$

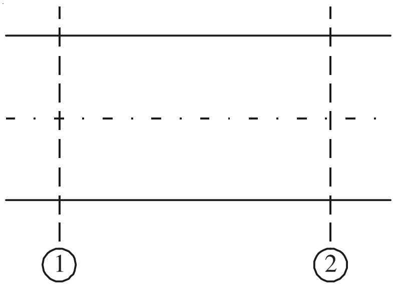
Equation 3.9-5 is a useful form of the engineering Bernoulli equation.

For design and operation, what is called the *friction factor approach* would be the easiest, with an acceptable balance between rigour and ease of usability. Let us use the friction factor approach for a few practical situations. As can be seen in the following sections, we invoke the just developed engineering Bernoulli equation quite extensively.

3.9.1 Friction Factor for Flow through a Straight Horizontal Pipe

Let us consider a well-developed flow through a straight horizontal pipe (Fig. 3.9.1-1).

Fig. 3.9.1-1 A section of the straight horizontal pipe taken for analysis



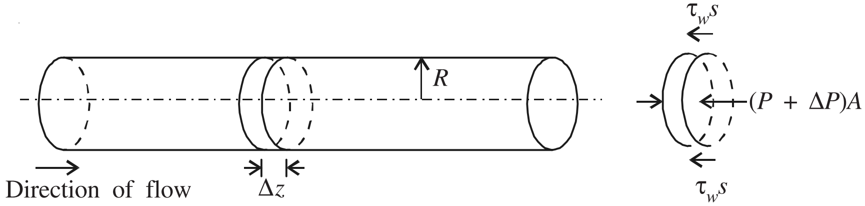


Fig. 3.9.1-2 Flow through a straight pipe, and a differential, disc-shaped fluid element taken for analysis

Let us apply the engineering Bernoulli equation between cross-sections 1 and 2

$$\frac{\Delta p}{\rho} + \overset{0(v_1 = v_2)}{\cancel{\frac{\Delta v^2}{2}}} + \overset{0(z_1 = z_2)}{\cancel{g\Delta z}} + \hat{F}_L + \overset{\text{no shaft work}}{\cancel{\hat{W}_s}} = 0$$

Thus

$$\widehat{FL} = -\frac{\Delta p}{\rho} \qquad (3.9.1\text{-}1)$$

Note that we have made no assumption regarding the nature of flow (i.e. whether it is laminar or turbulent). Thus, the above is applicable to both laminar and turbulent flows.

Let us consider a differential fluid volume which is disc-shaped of radius R and thickness, Δz, as shown in Fig. 3.9.1-2. τ_w will be the wall shear stress both in laminar and turbulent flows – this is because even in turbulent flow, the flow closest to the wall is laminar.

A force balance on the differential fluid element yields

$$p(\pi R^2) - (p + \Delta p)\,(\pi R^2) - \tau_\omega\,(2\pi R \Delta z) = 0 \qquad (3.9.1\text{-}2)$$

$$-\tau_\omega = \frac{(p+\Delta p)(\pi R^2) - p\pi R^2}{(\Delta z)(2\pi R)}$$

$$\tau_\omega = -\left(\frac{\Delta p}{\Delta z}\right)\frac{R}{2}$$

In the limit $\Delta z \to 0$

$$\tau_\omega = -\left(\frac{dp}{dz}\right)\frac{R}{2}$$

$$\frac{dp}{dz} + \frac{2\tau_\omega}{R} = 0 \tag{3.9.1-3}$$

For a pipe of length L between points 1 and 2, Eq. 3.9.1-3 can be integrated to yield

$$\frac{p_2 - p_1}{L} + \frac{2\tau_\omega}{R} = 0$$

or

$$\tau_\omega = \frac{-(p_2 - p_1)}{L} \times \frac{R}{2} = \frac{-(\Delta p)}{L} \times \frac{D}{4}$$

or

$$-\Delta p = \frac{4L\tau_\omega}{D}$$

Substituting this into Eq. 3.9.1-1, we get

$$\widehat{FL} = \frac{4\tau_\omega L}{\rho D} \tag{3.9.1-4}$$

Let us define a dimensionless parameter, f, as

$$f = \frac{(F_k)}{A} \times \frac{1}{KE'} \tag{3.9.1-5}$$

where f is the friction factor, F_k is the force exerted by a fluid due to its motion on the body of interest, A is the appropriate area and KE' is the kinetic energy per unit volume.

(A fluid exerts a force on a body in contact with it and of interest. That force can be thought to consist of two parts, F_s and F_k. F_s is the force that is exerted even when the fluid is stationary. F_k is the force exerted when the fluid is in relative motion compared to the body of interest.)

In our case of tube flow, f can be conveniently defined as

$$f \equiv \frac{\tau_\omega}{\left(\frac{1}{2}\right)\rho v_{\text{avg}}^2} = \frac{-\frac{\Delta p}{L} \times \frac{D}{4}}{\frac{1}{2}\rho v_{\text{avg}}^2} = \frac{(-\Delta p)D}{2L\rho v_{\text{avg}}^2} \tag{3.9.1-6}$$

Thus

$$\tau_\omega = \frac{1}{2}\rho v_{\text{avg}}^2 f \tag{3.9.1-7}$$

Substituting Eq. 3.9.1-7 in Eq. 3.9.1-4, we get

$$\widehat{FL} = \frac{4\left(\frac{1}{2}\rho v_{\text{avg}}^2 f\right)L}{\rho D} = 4f\left(\frac{L}{D}\right)\left(\frac{v_{\text{avg}}^2}{2}\right) \tag{3.9.1-8}$$

This $\widehat{FL}$ accounts for frictional losses at the pipe wall (skin friction). Equation 3.9.1-8 can be written as

$$\widehat{FL} = f\left(\frac{L}{\frac{D}{4}}\right)\left(\frac{v_{\text{avg}}^2}{2}\right)$$

If we define a 'hydraulic radius', r_H as

$$r_H = \frac{\text{Cross-sectional area}}{\text{Wetted perimeter}} \tag{3.9.1-9}$$

for our pipe

$$r_H = \frac{\pi\left(\frac{D^2}{4}\right)}{\pi D} = \frac{D}{4}$$

Thus

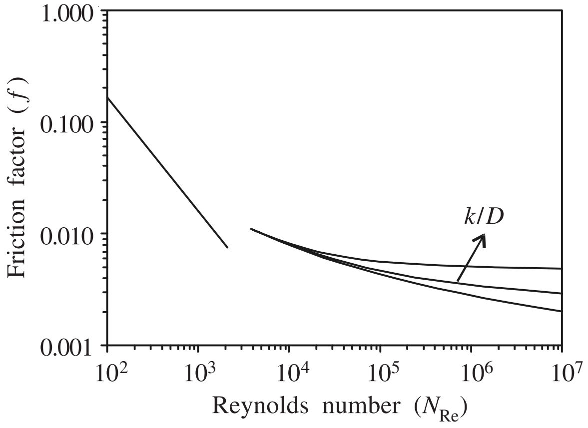
$$\widehat{FL} = f\left(\frac{L}{r_H}\right)\left(\frac{v_{\text{avg}}^2}{2}\right) \tag{3.9.1-10}$$

This equation, in practice, can be extended to all cross-sectional geometries.

To find the above friction factor for pipe flow, a friction factor chart (Fig. 3.9.1-3) can be used. The term 'friction factor' refers to the Fanning friction factor, and not the Moody's friction factor that is normally used in other (e.g. civil engineering) applications.

- For the laminar regions, we can use $f = \dfrac{16}{N_{\text{Re}}}$

Fig. 3.9.1-3 Friction factor chart



- For the turbulent regime, we need to use the chart.
- For the intermediate regime ($2100 < N_{\mathrm{Re}} < 4000$), we usually avoid design.

In the turbulent regime, the friction factor, f is a function of the roughness factor, k/D (represented as different curves on the friction factor chart), where k is the roughness length (effective thickness), and D is the diameter of the pipe.

The laminar region is represented by $f = \dfrac{16}{N_{\mathrm{Re}}}$. The turbulent region has different curves that correspond to different k/D values of the pipes. The lowest curve corresponds to a smooth pipe. The curve above that corresponds to a k/D of 10^{-4} and the topmost curve corresponds to a k/D value of 10^{-3}. For values in between, interpolations can be done to obtain estimates of f.

Example 3.9.1-1

A cleaning liquid used in many Bioprocess industries needs to be piped through the pipeline system above the ground as shown in Fig. 3.9.1-4.

The pipeline system consists of 50 m of 12" nominal diameter pipe and 20 m of 8" nominal diameter pipe. All elbows are standard and flanged, and the material used for the piping is schedule 80 wrought iron pipe. Determine the pressure drop needed between points 1 and 2 to maintain a flow rate of 0.05 $\mathrm{m^3 s^{-1}}$. What is the pumping power that is needed to maintain the flow rate? The density of the liquid is 870 kg $\mathrm{m^{-3}}$ and its viscosity is 1.375×10^{-3} Pa s.

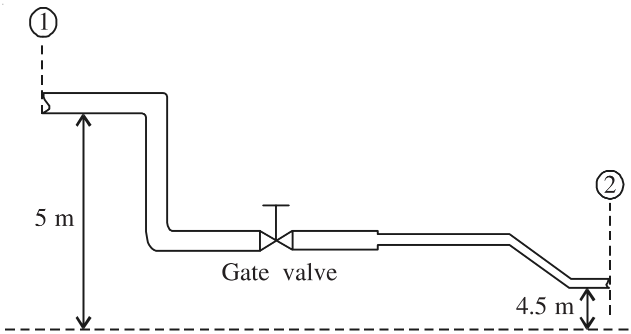


Fig. 3.9.1-4 Details of the pipeline for Example 3.9.1-1

Nominal diameter and schedule numbers are standard terminology used in process industries. They have evolved for historical reasons of communications between the different people working in the industry. The details of the terminology are given in various handbooks (e.g. *Perry's Chemical Engineers' Handbook* 2007) and other books too (McCabe et al. 2004).

In brief, the schedule number refers to the working stress and equals $1000\frac{p_{\max}}{S}$, where $p_{\max}$ is allowable working pressure and S is allowable tensile stress.

The correspondence between nominal diameter, internal diameter, and the wall thickness is available in many sources, e.g. the references given above.

For a 12" nominal diameter

$$\text{id} = 0.2889 \text{ m}$$
$$\therefore \text{ cs area} = 0.066 \text{ m}^2$$

For a 8" nominal diameter

$$\text{id} = 0.1937 \text{ m}$$
$$\therefore \text{ cs area} = 0.0297 \text{ m}^2$$

Also, for wrought iron, roughness factor (k) = 4.6×10^{-5} m.

Let us apply the engineering Bernoulli equation between points 1 and 2 in the piping network shown in Fig. 3.9.1-4.

$$\frac{\Delta P}{\rho} + \frac{\Delta v^2}{2} + g\Delta z + \hat{F}_L + \overset{0 \text{ (no shaft work)}}{\cancel{\hat{W}_s}} = 0$$

$$\frac{p_2 - p_1}{\rho} + \frac{(v_2^2 - v_1^2)}{2} + g(z_2 - z_1) + \widehat{FL} = 0$$

We need to find $p_2 - p_1$.

We know that $\rho = 870 \text{ kg m}^{-3}$

$$v_2 = \frac{\dot{V}_2}{A_2} = \frac{0.05}{0.0297} = 1.7 \text{ m s}^{-1}$$

$$v_1 = \frac{\dot{V}_1}{A_1} = \frac{0.05}{0.066} = 0.763 \text{ m s}^{-1}$$

$$z_2 = 4.5 \text{ m}; \; z_1 = 5 \text{ m}$$

$$\widehat{FL} = ?$$

For a pipe, and different pipe fittings (valves, etc., which are piping network components), $\widehat{FL}$ can be calculated as $\widehat{FL} = K_f \frac{v_{\text{avg}}^2}{2}$ for each fitting, and added together to get the total $\widehat{FL}$. K_f values for some common fittings are given in brackets next to the fitting: straight pipe $\left(4f\frac{L}{D}\right)$; 180° bend (2.2); 90° elbow (0.9); 45° elbow (0.4); tee (1.8); wide open globe valve (15); wide open gate valve (0.2). In addition, the K_f values for a sudden contraction and a sudden expansion can be evaluated as follows

$$\text{Sudden contraction: } 0.4\left(1 - \frac{A_b}{A_a}\right)$$

$$\text{Sudden expansion: } \left(1 - \frac{A_b}{A_a}\right)^2$$

where b is smaller diameter and a is larger diameter; v_{avg} is taken at b.

Thus, depending on the fittings in the piping network

$$\widehat{FL} = \left(4f\frac{L}{D} + \sum K_f\right)\frac{v_{\text{avg}}^2}{2}$$

In this case

$$\widehat{FL} = \sum K_f \frac{v_{\text{avg}}^2}{2}\bigg|_{12''} + 4f\frac{L}{D}\frac{v_{\text{avg}}^2}{2}\bigg|_{12''\text{ pipe}} + 4f\frac{L}{D}\frac{v_{\text{avg}}^2}{2}\bigg|_{8''\text{ pipe}} + \sum K_f \frac{v_{\text{avg}}^2}{2}\bigg|_{8''}$$

To find f, let us use the friction factor chart for which we need the Reynolds numbers.

$$N_{\text{Re},12''\text{ pipe}} = \frac{\rho v_{av} D}{\mu} = \frac{870 \times 0.763 \times 0.289}{1.375 \times 10^{-3}} = 1.39 \times 10^5$$

$$N_{\text{Re},8''\,\text{pipe}} = \frac{870\times 1.7\times 0.194}{1.375\times 10^{-3}} = 1.47\times 10^{5}$$

Both are turbulent flows.

Now, for reading the appropriate curve on the friction factor chart in the case of a turbulent flow, we need $\frac{k}{d}$.

$$\frac{k}{d_{12''}} = \frac{0.000046}{0.2889} = 1.6\times 10^{-4}$$

$$\frac{k}{d_{8''}} = \frac{0.000046}{0.194} = 2.37\times 10^{-4}$$

From the friction factor chart, $f_{12''} = 0.0045$; $f_{8''} = 0.00445$.

Pipe fittings: 2(12", 90°) + 2(8", 45°) elbows, 1(12") gate valve, 1(8") sudden contraction

$$\sum K_f\Big|_{12''} = 2\times 0.9 + 1\times 0.2 = 2.0$$

$$\sum K_f\Big|_{8''} = 2\times 0.4 + 0.4\left(1 - \frac{0.0297}{0.066}\right) = 1.02$$

Substituting the above in the engineering Bernoulli equation, we get

$$\frac{\Delta p}{870} + \frac{1.7^2 - 0.763^2}{2} + 9.8(45-5) + \left(4\times 0.0045\times\frac{50}{0.289}\times\frac{0.763^2}{2}\right)$$

$$+\left(4\times 0.0045\times\frac{20}{0.194}\times\frac{1.7^2}{2}\right) + \left(2\times\frac{0.763^2}{2}\right) + 1.02\times\frac{1.7^2}{2} = 0$$

$$\frac{\Delta p}{870} = 4.9 - 1.154 - 0.91 - 2.65 - 0.582 - 1.474$$

Δp = – 1626.9 Pa or – 1.63 kPa

Pumping power required

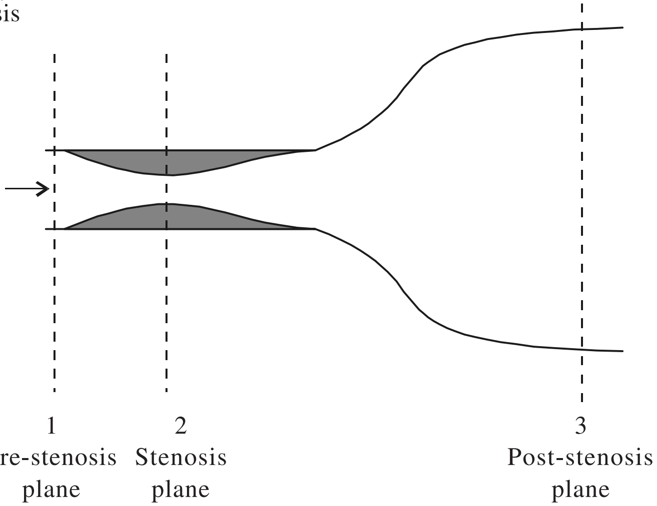
= $(-\Delta p)\times\dot{V}$

= 1626.9 × 0.05 = 81.3 W = 0.081 kW

Example 3.9.1-2

Stenosis or narrowing of the arteries can cause health difficulties especially cardiac related ones. If the stenosis happens to be at the place of expansion in

Fig. 3.9.1-5 Stenosis (narrowing) in an artery



the arterial cross-section, other difficulties could arise. One of the difficulties is due to “cavitation” or gas bubble formation followed by rupture. Rupture releases an enormous amount of energy that can even destroy metallic surfaces. Develop a criterion in terms of the flow velocities, pressure, and areas for the concept of cavitation at the stenosis.

Let us apply the engineering Bernoulli equation between planes 1 and 2 in Fig. 3.9.1-5. Upon cancelling the terms that are not relevant, we get

$$\frac{P_2-P_1}{\rho}+\frac{(v_{2,\text{avg}}^2-v_{1,\text{avg}}^2)}{2}+\overset{\substack{\text{(no change in}\\ \text{elevation)}\\ 0}}{\cancel{g\Delta z}}+\hat{F}_L+\overset{\text{0 (no shaft work)}}{\cancel{\hat{W}_s}}=0 \tag{3.9.1.2-1}$$

$\widehat{FL}$ here corresponds to the loss due to contraction. Approximating this contraction to a sudden contraction, from Example 3.9.1-1 we get

$$K_f=0.4\left(1-\frac{A_2}{A_1}\right)$$

where A is CS area.

Thus

$$\widehat{FL}=0.4\left(1-\frac{A_2}{A_1}\right)\frac{v_{2,\text{avg}}^2}{2}$$

Note the velocity we use here to calculate $\widehat{FL}$.

Thus

$$\frac{p_2 - p_1}{\rho} + \frac{(v_{2,\text{avg}}^2 - v_{1,\text{avg}}^2)}{2} + 0.4\left(1 - \frac{A_2}{A_1}\right)\frac{v_{2,\text{avg}}^2}{2} = 0 \qquad (3.9.1.2\text{-}2)$$

For cavitation to occur, bubbles of gas need to form or nucleation of gas bubbles need to take place. To understand the conditions for gas bubble formation, consider the case of boiling water. In boiling, bubbles begin to appear when the pressure increases due to temperature increase, and finally equals the saturated vapour pressure (note that this is not an equilibrium situation, and thus we cannot apply the phase diagram to find the relevant temperature-pressure relationship for the vapour and liquid phases). In the case of cavitation, the approach is from the other direction; the pressure decreases with increase in velocity of the fluid, and when the pressure equals or becomes lower than the saturated vapour pressure, bubbles form and cavitation occurs. Let us define the difference between the actual pressure and the saturated vapour pressure as p_g.

Thus

$$p_2 - p_1 = p_{2g} - p_{1g} \qquad (3.9.1.2\text{-}3)$$

Also for continuity

$$A_1 v_1 = A_2 v_2 \quad \text{or} \quad v_2 = \frac{A_1}{A_2} v_1 \qquad (3.9.1.2\text{-}4)$$

Since the pressure and velocity are inversely related, and since $v_2 > v_1$, $p_{g2} = 0$ is the condition for the onset of cavitation.

Substituting the above in Eq. 3.9.1.2-2, we get

$$-\frac{p_{g1}}{\rho} + \frac{1}{2} v_{1,\text{avg}}^2 \left(\frac{A_1^2}{A_2^2} - 1\right) + \frac{0.4}{2}\left(1 - \frac{A_2}{A_1}\right)\frac{A_1^2}{A_2^2} v_{1,\text{avg}}^2 = 0$$

$$-\frac{p_{g1}}{\rho} + \frac{v_{1,\text{avg}}^2}{2}\left(\frac{A_1^2}{A_2^2} - 1 + 0.4\frac{A_1^2}{A_2^2} - 0.4\frac{A_1}{A_2}\right) = 0$$

$$1.4\left(\frac{A_1}{A_2}\right)^2 - 0.4\left(\frac{A_1}{A_2}\right) - 1 = \frac{p_{g1}}{\rho} \times \frac{2}{v_{1,\text{avg}}^2}$$

$$1.4\left(\frac{A_1}{A_2}\right)^2 - 0.4\left(\frac{A_1}{A_2}\right) - \left(1 + \frac{p_{g1}}{\rho}\frac{2}{v_{1,\text{avg}}^2}\right) = 0$$

The solution of this quadratic equation provides the condition in terms of $\frac{A_1}{A_2}$ for cavitation to occur, i.e.

$$\frac{A_1}{A_2} = \frac{\left(0.4 \pm \sqrt{0.4^2 - 4 \times 1.4 \times \left(-1 + \frac{p_{g1}}{\rho} \times \frac{2}{v_{1,\text{avg}}^2}\right)}\right)}{2 \times 1.4}$$

$$= \frac{\left(0.4 \pm \sqrt{0.16 + 5.6\left(\frac{2p_{g1}}{\rho v_{1,\text{avg}}^2} - 1\right)}\right)}{2.8}$$

If $\frac{A_1}{A_2} \geq$ the above RHS, $p_{g2} \leq 0$, and cavitation will occur.

3.9.2 Friction Factor for Solids Moving Relative to a Fluid

For solids with a projected area, A_p (area projected on a plane that is normal to the relative motion direction)

$$F_k = (A_p)\left(\frac{1}{2}\rho v_\infty^2\right) f \qquad (3.9.2\text{-}1)$$

where v_∞ is the free stream velocity or the approach velocity at a large distance from the object.

F_k is often referred to as the drag force, while f is usually represented as C_D, the drag coefficient. A plot of variation of C_D with Reynolds number, N_{Re}, is available in handbooks, e.g. the one referred to in the earlier section.

When a sphere ($A_p = \pi R^2 = \pi D^2/4$) of density ρ_p falls through a fluid of density ρ, at a terminal velocity of v_t ($= v_\infty$), a simple force balance provides

$$F_k = \left(\frac{4}{3}\pi R^3\right)\rho_p g - \left(\frac{4}{3}\pi R^3\right)\rho g \qquad (3.9.2\text{-}2)$$

Using Eq. 3.9.2-1

$$F_k = (\pi R^2)\left(\frac{1}{2}\rho v_t^2\right) f$$

Equating the above two expressions, we can get an expression for the friction factor for this case, as

$$f = \frac{4}{3}\frac{gD}{v_t^2}\left(\frac{\rho_p - \rho}{\rho}\right) \qquad (3.9.2\text{-}3)$$

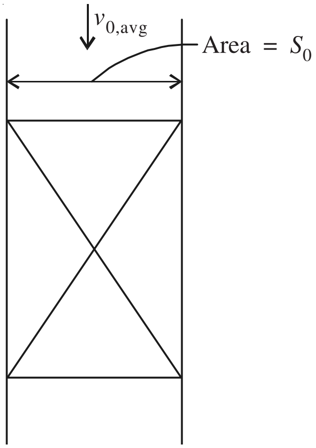


Fig. 3.9.3-1 A packed bed. $v_{0,\text{avg}}$ is average superficial velocity; the average velocity before the flow reaches the bed when there are no additional restrictions to flow

3.9.3 Friction Factor in Packed Beds

Packed beds are used in biological processes, especially in water and waste water processing. Certain stages of such processes involve removing undesirables by microorganisms or other agents in a packed bed.

A rigorous analysis of a packed bed is difficult, because even if an effort leads to a representative set of mathematical equations, they may not be easily solvable.

So, let us attempt a simpler analysis using the following assumptions:

- Replace the tortuous flow path inside the bed (Fig. 3.9.3-1) through the voids by a set of identical parallel conduits of the same length as that of the bed. Let the radius of each conduit be R, and the total cross-sectional area of the conduits (number of conduits times the CS area of each conduit) be S.
- Use a representative hydraulic radius to make the results somewhat extendable to many cross-sectional geometries.
- Let the particles be uniform with point contacts between them.
- Assume laminar flow in the conduits.

Let us consider that the total drag force (F_D) per unit total cross-sectional area in the parallel conduits is the sum of viscous drag forces (F_V), and inertial drag forces (F_I) per unit total CS area (S).

Now, let us focus our attention on each conduit with radius R, for a while. From Eq. 3.4.2-17 the average velocity in the conduit is

$$v_{\text{avg}} = \frac{(-\Delta P)R^2}{8\mu L} \tag{3.4.2-17}$$

We also know from the equation just before Eq. 3.9.1-4 that

$$(-\Delta P) = \frac{4L\tau_{w,V}}{D} \quad \text{or} \quad \frac{2L\tau_{w,V}}{R}$$

The subscript V refers to the viscous component. Substituting the above expression for $(-\Delta P)$ into Eq. 3.4.2-17, we get

$$v_{\text{avg}} = \left(\frac{2L\tau_{w,V}}{R}\right)\frac{R^2}{8\mu L}$$

Transposing, we get

$$\tau_{w,V} = \frac{4\mu v_{\text{avg}}}{R} \text{ and we know that } \tau_{w,V} = \frac{F_V}{S}$$

In terms of the hydraulic radius, r_H (to generalise it to channels of any cross-sectional shape)

$$\frac{F_V}{S} = \frac{k\mu v_{\text{avg}}}{r_H} \tag{3.9.3-1}$$

Now, let us look at the inertial component. The inertial force per unit cross-sectional area of the conduit

$$\frac{F_I}{S} = \tau_{w,I}$$

From Eq. 3.9.1-7, we get

$$\tau_{w,I} = \frac{1}{2}\rho v_{\text{avg}}^2 f = k_2\rho v_{\text{avg}}^2 \tag{3.9.3-2}$$

Thus, the total drag force per unit conduit area according to the summative consideration of the viscous and inertial components, is

$$\frac{F_D}{S} = \frac{k_1\mu v_{\text{avg}}}{r_H} + k_2\rho v_{\text{avg}}^2 \tag{3.9.3-3}$$

Now, let us focus on the entire bed. Let us define

$$\frac{\text{Volume of voids in the bed}}{\text{Total bed volume}} = \in \tag{3.9.3-4}$$

In other words

$$\frac{\text{CS area of imaginary conduits in bed} \times L_{\text{imaginary conduits}}}{\text{CS area of bed} \times L_{\text{bed}}} = \in$$

By one of our earlier assumptions

$$L_{\text{imaginary conduits}} = L_{\text{bed}}$$

Thus

$$\frac{\text{CS area of imaginary conduits in bed}}{\text{CS area of bed}} = \in \tag{3.9.3-5}$$

By mass conservation, since the mass flow rates through the conduits are additive, and S = total number of conduits × cross-sectional area of each conduit.

$$\rho v_{0,\text{avg}} S_0 = \rho v_{\text{avg}} S$$

Since the density is a constant

$$\frac{v_{0,\text{avg}}}{v_{\text{avg}}} = \frac{S}{S_0} = \in$$

or

$$v_{\text{avg}} = \frac{v_{0,\text{avg}}}{\in} \tag{3.9.3-6}$$

$v_{0,\text{avg}}$ i.e. 'superficial' or 'empty tower' velocity is much easier to measure compared to v_{avg}.

Now, let us relate the pressure drop across the bed to measurable parameters. To do that let us focus on the particles in the bed for a while. The aim is to express the relevant equations in terms of the measurable/calculable particle parameters.

The total surface area of the particles is A_S

$$A_s = N_p\ s_p \tag{3.9.3-7}$$

where N_p is total number of particles in the bed and s_p is area of one particle.

Assuming uniform particles

$$N_p \text{ is also} = \frac{\text{Volume of solids in bed}}{\text{Volume of one particle}} = \frac{S_0 L(1-\in)}{v_p} \tag{3.9.3-8}$$

where S_0 is cross-section of empty tower and L is bed length.

Substituting Eq. 3.9.3-7 in Eq. 3.9.3-8, we get

$$\frac{A_s}{s_p} = \frac{S_0 L(1-\in)}{v_p}$$

$$A_s = \frac{S_0 L(1-\in) s_p}{v_p} \tag{3.9.3-9}$$

Now

$$r_H = \frac{\text{CS area}}{\text{Wetted perimeter}} = \frac{\text{CS area} \times L}{\text{Wetted perimeter} \times L} = \frac{S\,L}{A_s} = \frac{(\in S_0)L}{A_s} \tag{3.9.3-10}$$

In the equation above, since we have assumed point contacts between particles, and hence there is no loss in surface area due to contact, the total surface area of the particles will equal the total surface area of the conduits.

Substituting A_s from Eq. 3.9.3-9 into Eq. 3.9.3-10, we get

$$r_H = \frac{\in S_0 L}{S_0 L(1-\in)\, s_p / v_p} = \frac{\in v_p}{(1-\in)s_p} \tag{3.9.3-11}$$

Substituting the above equation in Eq. 3.9.3-3, we get

$$F_D = \frac{S_0 \rho L(1-\in)s_p}{\in^2 v_p}\left[\frac{k_1 \mu v_{0,\text{avg}}(1-\in)s_p}{\rho v_p} + k_2 v_{0,\text{avg}}^2\right] \tag{3.9.3-12}$$

We can also express the drag force as the product of (pressure drop) and (effective area), i.e.

$$F_D = (-\Delta p)(S_0 \in)$$

Equating the two expressions for the drag force, we get

$$(-\Delta p)\, S_0 \in = S_0 \rho L\left(\frac{1-\in}{\in^2}\right)\left(\frac{s_p}{v_p}\right)\left[\frac{k_1 \mu v_{0,\text{avg}}(1-\in)s_p}{\rho v_p} + k_2 v_{0,\text{avg}}^2\right]$$

$$\frac{(-\Delta p)}{\rho L} = \left(\frac{1-\in}{\in^3}\right)\left(\frac{s_p}{v_p}\right)\left[\frac{k_1 \mu v_{0,\text{avg}}(1-\in)}{\rho}\,\frac{s_p}{v_p} + k_2 v_{0,\text{avg}}^2\right] \tag{3.9.3-13}$$

For a sphere

$$\frac{s_p}{v_p} = \frac{\pi D_p^2}{\frac{\pi}{6} D_p^3} = \frac{6}{D_p} \tag{3.9.3-14}$$

For any particle, let us define an equivalent diameter D_p as the diameter of the sphere having the same volume as that of the particle.

Let us also define sphericity, ϕ_s as

$$\phi_s = \frac{\text{Surface area of the equivalent sphere}}{\text{Actual surface area}} \tag{3.9.3-15}$$

$$\phi_s = \frac{\pi D_p^2}{s_p}$$

Thus

$$s_p = \frac{\pi D_p^2}{\phi_s}$$

and therefore

$$\therefore \frac{\Delta p}{v_p} = \frac{\pi D_p^2}{\phi_s \frac{\pi}{6} D_p^3} = \frac{6}{\phi_s D_p} \tag{3.9.3-16}$$

Values of ϕ_s for various commonly used particles are available in handbooks.

Ergun correlated experimental data and found that

$$k_1 = \frac{150}{36} \quad \text{and} \quad k_2 = \frac{1.75}{6}$$

Thus, the pressure drop equation can be written as

$$\frac{(-\Delta p)}{\rho v_{0,\text{avg}}^2} . \frac{\phi_s D_p}{L} . \frac{\in^3}{(1-\in)} = \frac{150}{\phi_s D_p} \frac{1-\in}{\rho v_{0,\text{avg}}^2 / \mu} + 1.75 \tag{3.9.3-17}$$

Equation 3.9.3-17 is called the Ergun equation. The above equation works well for most packings – except for packings of extreme shape such as needles, rings or saddles.

By comparison with the friction factor defined earlier, Eq. 3.9.1-6, we can define the friction factor for a packed bed as

$$f_{pb} \equiv \frac{(-\Delta p)\phi_s D_p \in^3}{\rho v_{0,\text{avg}}^2 L(1-\in)} \tag{3.9.3-18}$$

Substituting this back into Eq. 3.9.3-17, we get

$$f_{pb} = \frac{150(1-\in)}{\phi_s N_{\text{Re},p}} + 1.75 \tag{3.9.3-19}$$

At low $N_{\text{Re},p}$, 1.75 is negligible in comparison with the other term. Thus, at low $N_{\text{Re},p}$

$$f_{pb} = \frac{150(1-\in)}{\phi_s N_{\text{Re},p}} \tag{3.9.3-20}$$

This implies that (through substitution of the expression for f_{pb} back into the above equation)

$$\frac{(-\Delta p)\phi_s D_p^2 \in^3}{L v_{0,\text{avg}} \mu (1-\in)^2} = 150$$

$$(-\Delta p)\frac{S_0\phi_s D_p^2 \in^3}{S_0 v_{0,\text{avg}} L\mu(1-\in)^2} = 150$$

where $S_0 v_{0,\text{avg}}$ is volumetric flow rate, Q. The above equation is called the Kozeny-Carman equation.

If ϕ_s, D_p, and $\in$ are constants

$$Q \propto (-\Delta p) \text{ and } \propto \frac{1}{\mu L} \tag{3.9.3-21}$$

This is known as Darcy's law and has many applications.

At large N_{Re}, the first term in the RHS in Eq. 3.9.3-19 becomes negligible. Under such condition, we get the Blake-Plummer equation, i.e.

$$\frac{(-\Delta p)}{\rho v_{0,\text{avg}}^2}.\frac{\phi_s D_p}{L}.\frac{\in^3}{(1-\in)} = 1.75 \tag{3.9.3-22}$$

The above equations can be used to predict pressure drop across beds. Hence, the pumping requirements across packed beds can be estimated.

Exercises

1. Succinctly differentiate between

   (a) Laminar and turbulent flows
   (b) Pseudoplastic and dilatant fluids
   (c) Pseudoplastic and viscoelastic fluids
   (d) Bingham plastic and power law fluids
   (e) Viscosity and kinematic viscosity

2. Which model is an applicable constitutive equation for blood?

3. How do the equation of continuity in Chapter 2 and the equations of motion given in the tables in this chapter for laminar flow have to be modified so that they become applicable for turbulent flow?

4. There exists a concept called 'dynamic similarity' that makes it possible to use non-dimensional analysis for scale-up. Read up about the concept of dynamic similarity.

5. In a micro-processing unit for biological analytes that is based on microfluidics, multiple channels feed into a heating device that consists of a thin box-like structure with top and bottom faces that can be heated to increase the temperature of the fluid flowing through it. Even in the micro-dimensions,

the thickness of the box, *d*, or the space between the top and the bottom faces can be considered very small compared to the length and breadth of the heating box. An incompressible fluid of viscosity, μ, is flowing through it, and the heating is not turned on. If the pressure drop between the inlet and outlet of the heating box is a constant, *K*, derive an expression for the velocity profile of the fluid between the top and bottom faces of the boxes, when the flow is well developed; ignore entrance and exit effects. In a circular capillary section of the same set-up, what would be the flow rate, if the pressure due to surface tension is the only driving force for bulk flow in that section?

6. Two glass plates are placed horizontally at a distance of $3d$ from each other with a fluid in between them. A third thin rigid sheet (of negligible mass) is fixed between the plates, at a distance of d from the top plate – the sheet cannot move. The top plate is moved at a velocity of v ms^{-1}, and the bottom plate at 2 v ms^{-1}. Determine the velocity profiles at steady state when the plates are moved (a) in the same direction, and (b) in opposite directions.

7. It is well known that skiing in the snow-filled mountains in the northern regions of our country is possible because there is water formation from the snow/ice under the ski, due to pressure. This thin water layer provides the lubrication needed and makes skiing possible. Interestingly, it can be looked at as a water layer with the top part being bounded by the ski, and the bottom by the stationary solid ground (covered with snow/ice). Consider a person weighing 60 kg skiing on a 15° slope at a speed of 30 km h^{-1}. The ski bottom surface can be approximated to a rectangle of dimensions 14×80 cm^2. If the viscosity of water in the water layer is 1.8×10^{-3} N s m^{-2}, estimate the thickness of the water layer.

8. Set up the differential equations to obtain the velocity profile of a Newtonian fluid flowing in laminar flow, in a duct of square cross-section.

9. In one of our earlier studies in our lab that investigated the effects of a physical stress on the metabolic and genetic responses of cells, we needed to grow cells over extended periods at defined shear stress. We had used a co-axial cylinder set-up, and grew cells in the thin annular space between the cylinders. The outer cylinder was rotated at different rpms, thereby providing different shear rates, and hence different shear stresses on the cells. Develop expressions for the shear stress and the shear rate on the cells in terms of operational parameters, and discuss the expressions developed.

10. A lab deals with a particularly shear sensitive cell line which needs to be transported from one point to another in a pipe of length *L*, diameter, *D*. It was decided to use laminar flow for transport. Let the critical shear stress that the cells can tolerate be τ_{crit}, and the corresponding shear rate, assuming that the fluid is Newtonian be $\dot{\gamma}_{crit}$. Let the critical shear stress/rate be in the

range of shear that occurs in the laminar flow regime. Derive an expression for the maximum flow rate that can be used to transfer a uniform solution of the cells, of viscosity, μ, to ensure 80 % survival at the exit.

11. Semi-circular canals in the ear help the brain sense orientations of the head. They are three half-circular, inter-connected tubes inside the ear which are orthogonal (perpendicular) to each other. Each semi-circular canal is approximately a torus with a radius of curvature, say R, and inner radius of cross-section, a; $a << R$. Each canal is filled with a fluid called the endolymph, and contains a gelatinous membrane called cupula, a motion sensor with hair cells (cilia). The cilia move when the endolymph rushes past it and send a signal to the brain. The movement in the endolymph is induced as a result of twisting of the head. Hence a direct relation between angle of twist and cupula movement helps the brain sense rotations. The endolymph and cupula densities are constant and equal, under normal conditions, to avoid the effect of gravity on the cupula. Assume the endolymph to be Newtonian, with a density, r, and viscosity, n. Formulate a relationship between angular acceleration of the head with the rotation axis vertically located through the centre of the head, and cupula deflection in the corresponding semi-circular canal.

12. Atherosclerosis is a disease caused by the rise in the level of cholesterol in the body. The proteoglycans carried along the arteries are able to bind to the lining in the arteries. This leads to plaque build-up in the arteries, which results in the decrease of artery radius, and abnormal blood pressures. In a patient with atherosclerosis, the pressure drop in the artery, by some non-invasive method, was found to be $\Delta P'$, instead of ΔP under normal conditions. What is the thickness of the plaque built-up on the inner wall of the artery, if it can be assumed that the plaque covers the entire inner wall at the relevant region of the artery. Further assume that blood can be approximated to a Newtonian fluid for this purpose.

13. A student working on the SDS-page experiment prepared the required reagents for a stacking gel and kept it for his/her partner to process further. When the partner got to it after about 10 min, (s)he loaded the stacking gel into the pipette. Due to the time lapsed, the fluid behaves as a Bingham plastic now. Neglecting the tip of the pipette, find the steady state velocity profile in the pipette and the mass flow rate of the gel for a given constant pressure drop exerted by the mechanism in the pipette.

14. The lachrymal sac stores tears, and the tears flow through the lachrymal duct to the eye. By assuming that the lachrymal duct is a straight pipe of 12 mm length and 1 mm diameter, and by neglecting gravity, estimate the pressure needed to force the tears into the eyes through the larchrymal duct at a flow rate of 1.2 mL min^{-1} in laminar flow. Take the viscosity of the tears to be 4.4 Pa. s, and its density to be 1000 kg m^{-3}.

15. Pulsatile drug delivery systems have been used to deliver a desired amount of drug at the desired time and location. Develop an expression for the time dependent velocity of the drug solution for a given pressure drop, and other needed parameters.

Some of the exercise problems given above were suggested/formulated by G. Shashank, G. Vivek Sathvik, D. Divya Vani, I. Pradeep Kumar (6, 8), Akhil Sai Valluri (7), S. Kousik, Sagar Laygude, Utsav Saxena (10–12), Uma Maheswari, Namrata Kamat, Kiran, Kemun Khimun, Rashmi Kumari (13, 15), P. Raghavendran, P. Vivek, K. Ramasamy and M. Ashok (14).

Fully Open-ended Exercise

Estimate the power needed to overcome the frictional drag in the trachea. Use this to determine the efficiency of the trachea in the respiratory circuit, and propose an easily measurable physical parameter that can be used to decide whether a person with respiratory difficulties needs ventilator support. This problem was formulated by Akhil Sai Valluri, for his CFA exercise (CFA stands for choose-focus-analyse exercise). See end of Chapter 1 for some details.

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Part III
Energy Conservation

Chapter 4
Thermal Energy Flux

As we already know, the total energy in the universe is conserved. Let us now focus our attention on the transfer of energy as heat (thermal energy) across system boundaries, with the clarity that the thermal energy, a form of energy, is not conserved.

The transfer of heat due to molecular processes is called '*conduction*'. We have seen in the earlier chapters that constitutive equations govern some fluxes – Fick's first law governs diffusion (mass flux) and Newton's law governs laminar flow (momentum flux). Similarly, a constitutive equation known as 'Fourier's law' governs conduction (energy flux).

In one dimension, Fourier's law is written as

$$q_x = -k\frac{dT}{dx} \tag{4-1}$$

where q_x is heat flux in the x direction (units: J s^{-1} m^{-2}), T is temperature at position x (units: K) and k is thermal conductivity (units: J s^{-1} m^{-1} K).

The reader can learn about the methods to estimate thermal conductivity of gases and liquids in books like *Transport Phenomena*, Bird et al. (2002). In three dimensions, assuming an isotropic medium where the thermal conductivity is not a function of position, i.e. $k \neq f\,(x, y, z)$

$$\vec{q} = -k\vec{\nabla}T \tag{4-2}$$

In a moving fluid, $\vec{q}$ represents the flux of thermal energy relative to the local velocity. The equation for thermal energy flux in different coordinate systems is presented in Table 4-1.

Thermal diffusivity, α can be defined as

$$\alpha \equiv \frac{k}{\rho C_P} \tag{4-3}$$

Units of $\alpha = \dfrac{\cancel{\text{J}}\,\text{m}^{-1}\text{s}^{-1}\,\cancel{\text{K}^{-1}}}{\cancel{\text{kg}}\,\text{m}^{-3}\,\cancel{\text{J}\,\text{kg}^{-1}\,\text{K}^{-1}}} = \text{m}^2\text{s}^{-1}.$

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Table 4-1 Thermal energy flux (when only conduction is involved)

Rectangular

$$\vec{q} = -k\left[\frac{\partial T}{\partial x} + \frac{\partial T}{\partial y} + \frac{\partial T}{\partial z}\right] \tag{A}$$

Cylindrical

$$\vec{q} = -k\left[\frac{\partial T}{\partial r} + \frac{1}{r}\frac{\partial T}{\partial \theta} + \frac{\partial T}{\partial z}\right] \tag{B}$$

Spherical

$$\vec{q} = -k\left[\frac{\partial T}{\partial r} + \frac{1}{r}\frac{\partial T}{\partial \theta} + \frac{1}{r\sin\theta}\frac{\partial T}{\partial \phi}\right] \tag{C}$$

A comparison of α (heat) with D (mass) and $\nu = \frac{\mu}{\rho}$ (momentum) will show that all have the same units, and are comparable quantities in the three modes of fluxes.

4.1 Other Modes of Heat Flux

Heat flux due to molecular processes, or conduction, is only one of the modes for heat energy transport. For completeness, let us mention the other modes of heat flux – convection and radiation – here, with the understanding that we will learn about convection in detail in a later chapter. Radiation, on the other hand, is a different concept, and since it is difficult to slot radiation as a concept in the organisation of this book, let us discuss it in some detail in this section.

Flow induced heat flux is called *convection*. Convection could be of two kinds, forced convection and free convection. Forced convection occurs when heat is transferred due to flow generated by an external means such as a pressure gradient caused by a pump or a blower. Free convection occurs when heat is transferred due to a flow, normally small in magnitude, which is generated by a density differential, which in turn is caused by heating/cooling.

Heat flux can also occur due to *radiation*, which is mediated by electromagnetic waves. Simplistically speaking, as learnt in higher secondary school physics, the transitions of electrons between various energy levels in an atom result in emission of radiation. Thus, any substance at an absolute temperature of T K > 0 K will emit radiation over a range of wavelengths. Further, when any electromagnetic energy is incident on a substance, because of its electronic transitions, the substance will absorb the energy.

The Stefan-Boltzmann law that governs radiation states that the intensity of radiation is proportional to the fourth power of the temperature in K of the emitting body. When the energy is transferred as heat through radiation, from say, a body to its surroundings, the radiative flux can be expressed as

$$q_r = \sigma\,\varepsilon\left(T_{\text{body}}^4 - T_{\text{surr}}^4\right) \tag{4.1-1}$$

where σ, the Stefan-Boltzmann constant = 5.67×10^{-8} W m^{-2} K^{-4}, ε is emissivity of the body, and T is the absolute temperature. Radiative flux can dominate the heat transfer processes at high temperatures such as the ones that occur in steam-based heat exchangers in the bioprocess industries. An exercise problem at the end of this chapter will help the reader to get an idea of the relative contributions of conduction and radiation at physiological temperatures.

An aspect that needs important consideration in biological systems is that of phase change. If a phase change (e.g. evaporation of sweat) is involved, latent heat needs to be considered although it does not result in a temperature change.

We will consider some of the above concepts in the context of multiple driving forces and fluxes in Chapter 6.

4.2 Equation of Energy

As seen for mass and momentum transfer, although shell balances provided a physical feel for simple problems, the conservation equations were easier to employ for complex problems/situations, especially in coordinate systems other than rectangular.

Let us derive the equation of energy that can be applied in a heat transfer situation.

Consider the flow of a pure fluid through a stationary volume (control volume; the same as in Fig. 1.4.3-1). The various energies of relevance in this situation include the following:

- Internal energy, which can be visualised as arising from the vibrational, rotational, and potential energies of the molecules. Bird et al. (2002)

elegantly show how internal energy arises at the molecular level from the collision of two diatomic molecules, when the principle of energy conservation is invoked for the collision process.

- Kinetic energy, which is associated with the observable (bulk) motion.
- Potential energy (to begin with, it is clubbed with the 'work done' term because it can be interpreted as the work done against gravity).
- Other energies (say electrical, magnetic, surface, etc.), which we will ignore now – they can be added to the total energy term in the final equation by mere algebraic addition, if needed.

Let us also consider the other relevant terms that contribute to the overall energy balance over a (in our case, microscopic) control volume.

- Energy that crosses the control volume boundaries as heat through conduction.
- Energy that is generated as heat in the control volume by say, metabolic activities.
- Work done against stresses (and other aspects, such as gravity).

Then the law of conservation of energy can be written as

$$\begin{Bmatrix}\text{Rate of accumulation of}\\ \text{IE + KE in the system}\\ \text{or control volume}\end{Bmatrix}=\begin{Bmatrix}\text{Net rate of IE + KE}\\ \text{in by convection}\end{Bmatrix}$$

$$+\left\{\begin{matrix}\begin{Bmatrix}\text{Net rate of heat addition}\\ \text{by conduction}\end{Bmatrix}\\ +\begin{Bmatrix}\text{Net rate of heat addition by}\\ \text{generation, say metabolic}\end{Bmatrix}\end{matrix}\right\}$$

$$-\begin{Bmatrix}\text{Net work done by the system or}\\ \text{the control volume against}\\ \text{stress, gravity, etc.}\end{Bmatrix} \tag{4.2-1}$$

where IE is internal energy and KE is kinetic energy.

Now, let us take one term at a time from Eq. 4.2-1. Rate of accumulation of IE and KE is

$$(\Delta x\Delta y\Delta z)\frac{\partial}{\partial t}\left(\rho\hat{U}+\frac{1}{2}\rho v^2\right)$$

where $\hat{U}$ = IE per unit mass.

Net rate in of IE + KE by convection is

$$\Delta y \Delta z \left\{ v_x \left(\rho \hat{U} + \frac{1}{2}\rho v^2 \right)\bigg|_x - v_x \left(\rho \hat{U} + \frac{1}{2}\rho v^2 \right)\bigg|_{x+\Delta x} \right\}$$

$$+\Delta x \Delta z \left\{ v_y \left(\rho \hat{U} + \frac{1}{2}\rho v^2 \right)\bigg|_y - v_y \left(\rho \hat{U} + \frac{1}{2}\rho v^2 \right)\bigg|_{y+\Delta y} \right\}$$

$$+\Delta x \Delta y \left\{ v_z \left(\rho \hat{U} + \frac{1}{2}\rho v^2 \right)\bigg|_z - v_z \left(\rho \hat{U} + \frac{1}{2}\rho v^2 \right)\bigg|_{z+\Delta z} \right\}$$

Net rate in of Q by conduction is

$$\Delta y \Delta z\{q_x|_x - q_x|_{x+\Delta x}\} + \Delta x \Delta z\{q_y|_y - q_y|_{y+\Delta y}\} + \Delta x \Delta y\{q_z|_z - q_z|_{z+\Delta z}\}$$

where q_x, q_y and q_z are the components of the heat flux vector, $\vec{q}$.

Work done by the fluid element against its surroundings = work done against volume forces (gravity) + work done against surface forces (pressure, viscous forces) + other relevant work

Rate of work done against gravity is

$$-\ \rho(\Delta x \Delta y \Delta z)\ (v_x g_x + v_y g_y + v_z g_z)$$

Note:

1. Rate of work = Force × Velocity = Mass × Acceleration × Velocity
2. $\vec{v}$ and $\vec{g}$ have opposite signs

Rate of work done against the static pressure at the six faces is

$$\Delta y \Delta z\left\{(p v_x)|_{x+\Delta x} - (p v_x)|_x\right\} + \Delta x \Delta z\left\{(p v_y)|_{y+\Delta y} - (p v_y)|_y\right\}$$
$$+\ \Delta x \Delta y\left\{(p v_z)|_{z+\Delta z} - (p v_z)|_z\right\}$$

Rate of work done against viscous forces is

$$\Delta y \Delta z\left\{(\tau_{xx} v_x + \tau_{xy} v_y + \tau_{xz} v_z)|_{x+\Delta x} - (\tau_{xx} v_x + \tau_{xy} v_y + \tau_{xz} v_z)|_x\right\}$$

$$+\Delta x \Delta z\left\{(\tau_{yx} v_x + \tau_{yy} v_y + \tau_{yz} v_z)|_{y+\Delta y} - (\tau_{yx} v_x + \tau_{yy} v_y + \tau_{yz} v_z)|_y\right\}$$

$$+\Delta x \Delta y\left\{(\tau_{zx} v_x + \tau_{zy} v_y + \tau_{zz} v_z)|_{z+\Delta z} - (\tau_{zx} v_x + \tau_{zy} v_y + \tau_{zz} v_z)|_z\right\}$$

Let $\dot{W}_{\text{other}}$ be the other work interactions.

Substituting the above expressions into the energy balance (Eq. 4.2-1), dividing it by $\Delta x\Delta y\Delta z$ and taking the limit as $x \to 0$, $\Delta y \to 0$, $\Delta z \to 0$, we get

$$\begin{aligned}\frac{\partial}{\partial t}\left(\rho\hat{U}+\frac{1}{2}\rho v^2\right) = &-\left(\frac{\partial}{\partial x}v_x\left(\rho\hat{U}+\frac{1}{2}\rho v^2\right)+\frac{\partial}{\partial y}v_y\left(\rho\hat{U}+\frac{1}{2}\rho v^2\right)\right.\\ &\left.+\frac{\partial}{\partial z}v_z\left(\rho\hat{U}+\frac{1}{2}\rho v^2\right)\right)-\left(\frac{\partial q_x}{\partial x}+\frac{\partial q_y}{\partial y}+\frac{\partial q_z}{\partial z}\right)\\ &+\rho(v_x g_x+v_y g_y+v_z g_z)-\left(\frac{\partial}{\partial x}pv_x+\frac{\partial}{\partial y}pv_y+\frac{\partial}{\partial z}pv_z\right)\\ &-\left(\frac{\partial}{\partial x}(\tau_{xx}v_x+\tau_{xy}v_y+\tau_{xz}v_z)+\frac{\partial}{\partial y}(\tau_{yx}v_x+\tau_{yy}v_y+\tau_{yz}v_z)\right.\\ &\left.+\frac{\partial}{\partial z}(\tau_{zx}v_x+\tau_{zy}v_y+\tau_{zz}v_z)\right)\\ &+\dot{Q}_{\text{say, other like metabolic heat}}-\dot{W}_{\text{other}} \qquad (4.2\text{-}2)\end{aligned}$$

In vector notation

$$\begin{aligned}\underbrace{\frac{\partial}{\partial t}\rho\left(\hat{U}+\frac{1}{2}v^2\right)}_{\substack{\text{Rate of}\\ \text{energy}\\ \text{gain puv}}} = &\underbrace{-\left(\vec{\nabla}.\rho\vec{v}\left(\hat{U}+\frac{1}{2}v^2\right)\right)}_{\substack{\text{Rate of}\\ \text{energy in, puv}\\ \text{by convection}}} \underbrace{-(\vec{\nabla}.\vec{q})}_{\substack{\text{Rate of}\\ \text{energy in, puv}\\ \text{by conduction}}} \underbrace{+\rho(\vec{v}.\vec{g})}_{\substack{\text{Rate of work}\\ \text{done on the}\\ \text{fluid puv by}\\ \text{gravitational forces}}}\\ &\underbrace{-(\vec{\nabla}.p\vec{v})}_{\substack{\text{Rate of work done}\\ \text{on the fluid puv by}\\ \text{pressure forces}}} \underbrace{-(\vec{\nabla}.[\tilde{\tau}.\vec{v}])}_{\substack{\text{Rate of work done}\\ \text{on the fluid puv by}\\ \text{viscous forces}}}\\ &+\dot{Q}_{\text{say, other like metabolic heat}}-\dot{W}_{\text{other}} \qquad (4.2\text{-}3)\end{aligned}$$

where puv is per unit volume.

Now, let us consider the LHS of the above equation (by transposition) as

$$\frac{\partial\rho}{\partial t}\left(\hat{U}+\frac{1}{2}v^2\right)+\left(\vec{\nabla}\cdot\rho\vec{v}\left(\hat{U}+\frac{1}{2}v^2\right)\right)$$

We know that (see Appendix 1)

$$\vec{\nabla} rs = r\vec{\nabla} s + s\vec{\nabla} r$$

and

$$\vec{\nabla}\cdot s\vec{v} = s\vec{\nabla}\cdot\vec{v} + \vec{v}\cdot\vec{\nabla} s$$

Therefore

$$\begin{aligned}\vec{\nabla}\cdot rs\vec{v} &= \vec{v}\cdot\vec{\nabla} rs + rs\vec{\nabla}\cdot\vec{v}\\ &= \vec{v}\cdot(r\vec{\nabla} s + s\vec{\nabla} r) + rs\vec{\nabla}\cdot\vec{v}\end{aligned}$$

Thus, the above expression can be written as

$$\rho\frac{\partial}{\partial t}\left(\hat{U}+\frac{1}{2}v^2\right)+\left(\hat{U}+\frac{1}{2}v^2\right)\frac{\partial\rho}{\partial t}+\left(\vec{\nabla}\cdot\rho\vec{v}\left(\hat{U}+\frac{1}{2}v^2\right)\right)$$

$$\begin{aligned}&=\rho\frac{\partial}{\partial t}\left(\hat{U}+\frac{1}{2}v^2\right)+\left(\hat{U}+\frac{1}{2}v^2\right)\frac{\partial\rho}{\partial t}\\ &\quad+\vec{v}\cdot\left(\rho\vec{\nabla}\left(\hat{U}+\frac{1}{2}v^2\right)+\left(\hat{U}+\frac{1}{2}v^2\right)\vec{\nabla}\rho\right)+\rho\left(\hat{U}+\frac{1}{2}v^2\right)\vec{\nabla}\cdot\vec{v}\end{aligned}$$

$$=\rho\left(\frac{\partial}{\partial t}\left(\hat{U}+\frac{1}{2}v^2\right)+\vec{v}\cdot\vec{\nabla}\left(\hat{U}+\frac{1}{2}v^2\right)\right)+\left(\hat{U}+\frac{1}{2}v^2\right)\left\{\frac{\partial\rho}{\partial t}+\vec{v}\cdot\vec{\nabla}\rho+\rho\vec{\nabla}\cdot\vec{v}\right\}$$

$$=\rho\left(\frac{\partial}{\partial t}\left(\hat{U}+\frac{1}{2}v^2\right)+\vec{v}\cdot\vec{\nabla}\left(\hat{U}+\frac{1}{2}v^2\right)\right)+\left(\hat{U}+\frac{1}{2}v^2\right)\left\{\cancelto{0}{\frac{\partial\rho}{\partial t}+\vec{\nabla}\cdot\rho\vec{v}}\right\}$$

The last term goes to zero according to the equation of continuity.

Thus, the expression becomes

$$\rho\left(\frac{\partial}{\partial t}\left(\hat{U}+\frac{1}{2}v^2\right)+\vec{v}\cdot\vec{\nabla}\left(\hat{U}+\frac{1}{2}v^2\right)\right)=\rho\left(\frac{D}{Dt}\left(\hat{U}+\frac{1}{2}v^2\right)\right)$$

Therefore, the energy equation can be written as

$$\rho\left(\frac{D}{Dt}\left(\hat{U}+\frac{1}{2}v^2\right)\right)=-(\vec{\nabla}\cdot\vec{q})+\rho(\vec{v}\cdot\vec{g})-(\vec{\nabla}\cdot p\vec{v})-(\vec{\nabla}\cdot[\tilde{\tau}\cdot\vec{v}])+\dot{Q}_{\text{other}}-\dot{W}_{\text{other}} \tag{4.2-4}$$

In the rate of heat term, $\dot{Q}_{\text{other}}$, the 'other' could refer to metabolic heat.

Earlier, to derive the equation of mechanical energy, we considered the potential energy contribution in the 'work done' term. If the external force per unit mass, $\vec{g}$, is expressible as a gradient of a scalar function, i.e.

$$\vec{g} = -\vec{\nabla}\phi \qquad (4.2\text{-}5)$$

Then

$$\rho(\vec{v}\cdot\vec{g}) = -\rho(\vec{v}\cdot\vec{\nabla}\phi)$$

From the identity

$$\frac{Ds}{Dt} = \frac{ds}{dt} + (\vec{v}\cdot\vec{\nabla}s)$$

we can write

$$-\rho(\vec{v}\cdot\vec{\nabla}\phi) = -\rho\left(\frac{D\phi}{Dt} - \frac{d\phi}{dt}\right)$$

If ϕ is time independent, as for all terrestrial cases, then, $\dfrac{d\phi}{dt} = 0$. However, note that $\dfrac{D\phi}{Dt} \neq 0$ because it involves the variation with spatial variables too. Thus

$$\rho\frac{D}{Dt}\left(\hat{U} + \phi + \frac{1}{2}v^2\right) = -(\vec{\nabla}\cdot\vec{q}) - (\vec{\nabla}\cdot p\vec{v}) - (\vec{\nabla}\cdot[\tilde{\tau}\cdot\vec{v}]) + \dot{Q}_{\text{other}} - \dot{W}$$

Note that the last term, the rate of work, $\dot{W}$, does not include the gravitational work.

Many applications require the consideration of thermal energy alone – let us focus more on that now. Note that thermal energy is not conserved. However, a suitable expression can be developed in terms of thermal energy alone.

To arrive at this useful expression involving only thermal energy, let us begin with Eq. 4.2-4. We need to get rid of the kinetic energy term and be left only with the internal energy (thermal) term in Eq. 4.2-4. To do that, let us consider Eq. 3.4-5, the equation of motion.

$$\rho\frac{D\vec{v}}{Dt} = -[\vec{\nabla}\cdot\tilde{\tau}] - \vec{\nabla}p + \rho\vec{g} \qquad (3.4\text{-}5)$$

If we take the dot product of every term in Eq. 3.4-5 with the velocity vector, we get

$$\vec{v}\cdot\rho\frac{D\vec{v}}{Dt} = -(\vec{v}\cdot[\vec{\nabla}\cdot\tilde{\tau}]) - (\vec{v}\cdot\vec{\nabla}p) + (\vec{v}\cdot\rho\vec{g})$$

which can be written as

$$\rho\frac{D}{Dt}\left(\frac{1}{2}v^2\right) = -(\vec{v}\cdot[\vec{\nabla}\cdot\tilde{\tau}]) - (\vec{v}\cdot\vec{\nabla}p) + (\vec{v}\cdot\rho\vec{g}) \qquad (4.2\text{-}6)$$

If we subtract Eq. 4.2-5 from Eq. 4.2-4, we get

$$\rho\frac{D}{Dt}(\hat{U}) = -(\vec{\nabla}\cdot\vec{q}) + \rho(\vec{v}\cdot\vec{g}) - (\vec{\nabla}\cdot p\vec{v}) - (\vec{\nabla}\cdot[\tilde{\tau}\cdot\vec{v}]) + \dot{Q}_{\text{other}} - \dot{W}_{\text{other}}$$

$$+(\vec{v}\cdot[\vec{\nabla}\cdot\tilde{\tau}]) + (\vec{v}\cdot\vec{\nabla}p) - (\vec{v}\cdot\rho\,\vec{g}) \tag{4.2-7}$$

Using the chain rule, we can combine the third and the eighth terms on the RHS as

$$(\vec{v}\cdot\vec{\nabla}p) - (\vec{\nabla}\cdot p\vec{v}) = -p(\vec{\nabla}\cdot\vec{v})$$

The second and the last terms in the RHS of Eq. 4.2-7 can be cancelled with each other, and it can be shown (students are encouraged to show this) that

$$(\vec{v}\cdot[\vec{\nabla}\cdot\tilde{\tau}]) - (\vec{\nabla}\cdot[\tilde{\tau}\cdot\vec{v}]) = -(\tilde{\tau}:\vec{\nabla}\vec{v})$$

where ':' is a scalar product between two tensors or equivalents. For example, the ':' product between $\tilde{\tau}$ and $\vec{\nabla}\vec{v}$ (note that both have 9 components, each, in a 3-D system) is the scalar given by

$$\tau_{xx}\left(\frac{\partial v_x}{\partial x}\right) + \tau_{xy}\left(\frac{\partial v_x}{\partial y}\right) + \tau_{xz}\left(\frac{\partial v_x}{\partial z}\right)$$

$$+\tau_{yx}\left(\frac{\partial v_y}{\partial x}\right) + \tau_{yy}\left(\frac{\partial v_y}{\partial y}\right) + \tau_{yz}\left(\frac{\partial v_y}{\partial z}\right)$$

$$+\tau_{zx}\left(\frac{\partial v_z}{\partial x}\right) + \tau_{zy}\left(\frac{\partial v_z}{\partial y}\right) + \tau_{zz}\left(\frac{\partial v_z}{\partial z}\right)$$

Thus, we can write Eq. 4.2-7 as

$$\rho\frac{D}{Dt}(\hat{U}) = -(\vec{\nabla}\cdot\vec{q}) - p(\vec{\nabla}\cdot\vec{v}) - (\tilde{\tau}:\vec{\nabla}\vec{v}) + \dot{Q}_{\text{other}} - \dot{W}_{\text{other}} \tag{4.2-8}$$

Since $\hat{U}$ is not easily measurable, it may be preferable to rewrite the expressions in terms of more easily measurable variables such as p, T, C_V, etc. We know from thermodynamics that when we consider $\hat{U} = f(\hat{V},T)$, where $\hat{U}$ is the mass specific internal energy, and $\hat{V}$ is the mass specific volume (inverse of density), we can write

$$d\hat{U} = \left(\frac{\partial\hat{U}}{\partial\hat{V}}\right)_T d\hat{V} + \left(\frac{\partial\hat{U}}{\partial T}\right)_{\hat{V}} dT$$

We also know from thermodynamics that

$$\left(\frac{\partial \hat{U}}{\partial \hat{V}}\right)_T = \left(-p + T\left(\frac{\partial p}{\partial T}\right)_{\hat{V}}\right)$$

Therefore

$$d\hat{U} = \left(-p + T\left(\frac{\partial p}{\partial T}\right)_{\hat{V}}\right) d\hat{V} + C_V \, dT \tag{4.2-9}$$

If we take the substantial derivative of the above equation, and multiply throughout by ρ, we get

$$\rho \frac{D\hat{U}}{Dt} = \left(-p + T\left(\frac{\partial p}{\partial T}\right)_{\hat{V}}\right) \rho \frac{D\hat{V}}{Dt} + \rho\, C_V \frac{DT}{Dt} \tag{4.2-10}$$

Now

$$\rho \frac{D\hat{V}}{Dt} = \rho \frac{D\left(\dfrac{1}{\rho}\right)}{Dt} = -\left(\frac{1}{\rho}\right)\frac{D\rho}{Dt}$$

From the equation of continuity, Eq. 1.4.3-7, we can write

$$-\left(\frac{1}{\rho}\right)\frac{D\rho}{Dt} = (\vec{\nabla} \cdot \vec{v})$$

Thus, we can write Eq. 4.2-10 as

$$\rho \frac{D\hat{U}}{Dt} = \left(-p + T\left(\frac{\partial p}{\partial T}\right)_{\hat{V}}\right)(\vec{\nabla} \cdot \vec{v}) + \rho\, C_V \frac{DT}{Dt} \tag{4.2-11}$$

Substituting Eq. 4.2-11 into the LHS of Eq. 4.2-8, we get

$$\left(-p + T\left(\frac{\partial p}{\partial T}\right)_{\hat{V}}\right)(\vec{\nabla} \cdot \vec{v}) + \rho C_V \frac{DT}{Dt} = -(\vec{\nabla} \cdot \vec{q}) - p(\vec{\nabla} \cdot \vec{v}) - (\tilde{\tau} : \vec{\nabla}\vec{v}) + \dot{Q}_{\text{other}} - \dot{W}_{\text{other}}$$

Since the first part of the first term on the LHS of the above equation cancels with the second term on the RHS of the same equation, the equation can be rewritten as

$$\rho C_V \frac{DT}{Dt} = -(\vec{\nabla} \cdot \vec{q}) - T\left(\frac{\partial p}{\partial T}\right)_{\hat{V}} (\vec{\nabla} \cdot \vec{v}) - (\tilde{\tau} : \vec{\nabla}\vec{v}) + \dot{Q}_{\text{other}} - \dot{W}_{\text{other}} \tag{4.2-12}$$

The above equation, which is useful when thermal energy alone needs to be considered (although it is not conserved), is given in Table 4.2-1 in various coordinate systems.

Table 4.2-1 The equation of thermal energy

Rectangular coordinate system

$$
\begin{aligned}
&\rho C_V\left(\frac{\partial T}{\partial t}+v_x\frac{\partial T}{\partial x}+v_y\frac{\partial T}{\partial y}+v_z\frac{\partial T}{\partial z}\right)\\
&\quad=-\left[\frac{\partial q_x}{\partial x}+\frac{\partial q_y}{\partial y}+\frac{\partial q_z}{\partial z}\right]\\
&\qquad-T\left(\frac{\partial p}{\partial T}\right)_\rho\left(\frac{\partial v_x}{\partial x}+\frac{\partial v_y}{\partial y}+\frac{\partial v_z}{\partial z}\right)-\left\{\tau_{xx}\left(\frac{\partial v_x}{\partial x}\right)+\tau_{yy}\left(\frac{\partial v_y}{\partial y}\right)+\tau_{zz}\left(\frac{\partial v_z}{\partial z}\right)\right\}\\
&\qquad-\left\{\tau_{xy}\left(\frac{\partial v_x}{\partial y}+\frac{\partial v_y}{\partial x}\right)+\tau_{xz}\left(\frac{\partial v_x}{\partial z}+\frac{\partial v_z}{\partial x}\right)+\tau_{yz}\left(\frac{\partial v_y}{\partial z}+\frac{\partial v_z}{\partial y}\right)\right\}\\
&\qquad+\dot{Q}_{\text{other}}-\dot{W}_{\text{other}}
\end{aligned}
\tag{A1}
$$

For a Newtonian fluid, when ρ and k are constant

$$
\begin{aligned}
&\rho C_V\left(\frac{\partial T}{\partial t}+v_x\frac{\partial T}{\partial x}+v_y\frac{\partial T}{\partial y}+v_z\frac{\partial T}{\partial z}\right)\\
&\quad=k\left[\frac{\partial^2 T}{\partial x^2}+\frac{\partial^2 T}{\partial y^2}+\frac{\partial^2 T}{\partial z^2}\right]+2\mu\left\{\left(\frac{\partial v_x}{\partial x}\right)^2+\left(\frac{\partial v_y}{\partial y}\right)^2+\left(\frac{\partial v_z}{\partial z}\right)^2\right\}\\
&\quad+\mu\left\{\left(\frac{\partial v_x}{\partial y}+\frac{\partial v_y}{\partial x}\right)^2+\left(\frac{\partial v_x}{\partial z}+\frac{\partial v_z}{\partial x}\right)^2+\left(\frac{\partial v_y}{\partial z}+\frac{\partial v_z}{\partial y}\right)^2\right\}+\dot{Q}_{\text{other}}-\dot{W}_{\text{other}}
\end{aligned}
\tag{A2}
$$

Cylindrical coordinate system

$$
\begin{aligned}
&\rho C_V\left(\frac{\partial T}{\partial t}+v_r\frac{\partial T}{\partial r}+\frac{v_\theta}{r}\frac{\partial T}{\partial \theta}+v_z\frac{\partial T}{\partial z}\right)\\
&\quad=-\left[\frac{1}{r}\frac{\partial}{\partial r}(rq_r)+\frac{1}{r}\frac{\partial q_\theta}{\partial \theta}+\frac{\partial q_z}{\partial z}\right]-T\left(\frac{\partial p}{\partial T}\right)_\rho\left(\frac{1}{r}\frac{\partial}{\partial r}(rv_r)+\frac{1}{r}\frac{\partial v_\theta}{\partial \theta}+\frac{\partial v_z}{\partial z}\right)\\
&\qquad-\left\{\tau_{rr}\frac{\partial v_r}{\partial r}+\tau_{\theta\theta}\frac{1}{r}\left(\frac{\partial v_\theta}{\partial \theta}+v_r\right)+\tau_{zz}\frac{\partial v_z}{\partial z}\right\}\\
&\qquad-\left\{\tau_{r\theta}\left[r\frac{\partial}{\partial r}\left(\frac{v_\theta}{r}\right)+\frac{1}{r}\frac{\partial v_r}{\partial \theta}\right]+\tau_{rz}\left(\frac{\partial v_z}{\partial r}+\frac{\partial v_r}{\partial z}\right)+\tau_{\theta z}\left(\frac{1}{r}\frac{\partial v_z}{\partial \theta}+\frac{\partial v_\theta}{\partial z}\right)\right\}\\
&\quad+\dot{Q}_{\text{other}}-\dot{W}_{\text{other}}
\end{aligned}
\tag{B1}
$$

For a Newtonian fluid, when ρ and k are constant

$$
\rho C_V\left(\frac{\partial T}{\partial t}+v_r\frac{\partial T}{\partial r}+\frac{v_\theta}{r}\frac{\partial T}{\partial \theta}+v_z\frac{\partial T}{\partial z}\right)
$$

Contd…

Table 4.2-1 Continued

$$
\begin{aligned}
&= k\left[\frac{1}{r}\frac{\partial}{\partial r}\left(r\frac{\partial T}{\partial r}\right)+\frac{1}{r^2}\frac{\partial^2 T}{\partial \theta^2}+\frac{\partial^2 T}{\partial z^2}\right]+2\mu\left\{\left(\frac{\partial v_r}{\partial r}\right)^2+\left[\frac{1}{r}\left(\frac{\partial v_\theta}{\partial \theta}+v_r\right)\right]^2+\left(\frac{\partial v_z}{\partial z}\right)^2\right\}\\
&+\mu\left\{\left(\frac{\partial v_\theta}{\partial z}+\frac{1}{r}\frac{\partial v_z}{\partial \theta}\right)^2+\left(\frac{\partial v_z}{\partial r}+\frac{\partial v_r}{\partial z}\right)^2+\left[\frac{1}{r}\frac{\partial v_r}{\partial \theta}+r\frac{\partial}{\partial r}\left(\frac{v_\theta}{r}\right)\right]^2\right\}\\
&+\dot{Q}_{\text{other}}-\dot{W}_{\text{other}}
\end{aligned}
\tag{B2}
$$

Spherical coordinate system

$$
\begin{aligned}
&\rho C_V\left(\frac{\partial T}{\partial t}+v_r\frac{\partial T}{\partial r}+\frac{v_\theta}{r}\frac{\partial T}{\partial \theta}+\frac{v_\phi}{r\sin\theta}\frac{\partial T}{\partial \phi}\right)\\
&=-\left[\frac{1}{r^2}\frac{\partial}{\partial r}(r^2 q_r)+\frac{1}{r\sin\theta}\frac{\partial}{\partial \theta}(q_\theta\sin\theta)+\frac{1}{r\sin\theta}\frac{\partial q_\phi}{\partial \phi}\right]\\
&-T\left(\frac{\partial p}{\partial T}\right)_\rho\left(\frac{1}{r^2}\frac{\partial}{\partial r}(r^2 v_r)+\frac{1}{r\sin\theta}\frac{\partial}{\partial \theta}(v_\theta\sin\theta)+\frac{1}{r\sin\theta}\frac{\partial v_\phi}{\partial \phi}\right)\\
&-\left\{\tau_{rr}\frac{\partial v_r}{\partial r}+\tau_{\theta\theta}\frac{1}{r}\left(\frac{\partial v_\theta}{\partial \theta}+\frac{v_r}{r}\right)+\tau_{\phi\phi}\left(\frac{1}{r\sin\theta}\frac{\partial v_\phi}{\partial \phi}+\frac{v_r}{r}+\frac{v_\theta\cot\theta}{r}\right)\right\}\\
&-\left\{\tau_{r\theta}\left(\frac{\partial v_\theta}{\partial r}+\frac{1}{r}\frac{\partial v_r}{\partial \theta}-\frac{v_\theta}{r}\right)+\tau_{r\phi}\left(\frac{\partial v_\phi}{\partial r}+\frac{1}{r\sin\theta}\frac{\partial v_r}{\partial \phi}-\frac{v_\phi}{r}\right)\right.\\
&\left.+\tau_{\theta\phi}\left(\frac{1}{r}\frac{\partial v_\phi}{\partial \theta}+\frac{1}{r\sin\theta}\frac{\partial v_\theta}{\partial \phi}-\frac{v_\phi\cot\theta}{r}\right)\right\}+\dot{Q}_{\text{other}}-\dot{W}_{\text{other}}
\end{aligned}
\tag{C1}
$$

For a Newtonian fluid, when ρ and *k* are constant

$$
\begin{aligned}
&\rho C_V\left(\frac{\partial T}{\partial t}+v_r\frac{\partial T}{\partial r}+\frac{v_\theta}{r}\frac{\partial T}{\partial \theta}+\frac{v_\phi}{r\sin\theta}\frac{\partial T}{\partial \phi}\right)\\
&=k\left[\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial T}{\partial r}\right)+\frac{1}{r^2\sin\theta}\frac{\partial}{\partial \theta}\left(\sin\theta\frac{\partial T}{\partial \theta}\right)+\frac{1}{r^2\sin^2\theta}\frac{\partial^2 T}{\partial \phi^2}\right]\\
&+2\mu\left\{\left(\frac{\partial v_r}{\partial r}\right)^2+\left[\frac{1}{r}\frac{\partial v_\theta}{\partial \theta}+\frac{v_r}{r}\right]^2+\left(\frac{1}{r\sin\theta}\frac{\partial v_\phi}{\partial \phi}+\frac{v_r}{r}+\frac{v_\theta\cot\theta}{r}\right)^2\right\}\\
&+\mu\left\{\left(r\frac{\partial}{\partial r}\left(\frac{v_\theta}{r}\right)+\frac{1}{r}\frac{\partial v_r}{\partial \theta}\right)^2+\left(\frac{1}{r\sin\theta}\frac{\partial v_r}{\partial \phi}+r\frac{\partial}{\partial r}\left(\frac{v_\phi}{r}\right)\right)^2\right.\\
&\left.+\left[\frac{\sin\theta}{r}\frac{\partial}{\partial \theta}\left(\frac{v_\phi}{\sin\theta}\right)+\frac{1}{r\sin\theta}\frac{\partial v_\theta}{\partial \phi}\right]^2\right\}+\dot{Q}_{\text{other}}-\dot{W}_{\text{other}}
\end{aligned}
\tag{C2}
$$

In many situations, it has been found that it is more convenient to work with C_p rather than with C_V. If Eq. 4.2-8 can be written in terms of specific enthalpy, instead of in terms of specific internal energy, the use of C_p can be facilitated. To do this, let us recognise that by definition

$$\hat{H} = \hat{U} + P\hat{V} = \hat{U} + \frac{p}{\rho}$$

Thus, Eq. 4.2-8 can be written as

$$\rho \frac{D}{Dt}\left(\hat{H} - \frac{p}{\rho}\right) = -(\vec{\nabla}\cdot\vec{q}) - p(\vec{\nabla}\cdot\vec{v}) - (\tilde{\tau}:\vec{\nabla}\vec{v}) + \dot{Q}_{\text{other}} - \dot{W}_{\text{other}} \tag{4.2-13}$$

The LHS of Eq. 4.2-13 becomes

$$\rho\left\{\frac{D\hat{H}}{Dt} - \left(\frac{\rho\frac{Dp}{Dt} - p\frac{D\rho}{Dt}}{\rho^2}\right)\right\}$$

$$= \rho\frac{D\hat{H}}{Dt} - \frac{Dp}{Dt} + \frac{p}{\rho}\frac{D\rho}{Dt} \tag{4.2-14}$$

On the same lines as we developed earlier, after Eq. 4.2-8, taking $\hat{H} = f(T, p)$, we can write

$$d\hat{H} = \left(\frac{\partial \hat{H}}{\partial T}\right)_p dT + \left(\frac{\partial \hat{H}}{\partial p}\right)_T dp$$

By substituting the relations we know from thermodynamics, we get

$$d\hat{H} = C_p dT + \left[\hat{V} - T\left(\frac{\partial \hat{V}}{\partial T}\right)_p\right] dp \tag{4.2-15}$$

If we take the substantial derivative, and multiply throughout by ρ, we get

$$\rho\frac{D\hat{H}}{Dt} = \rho C_p \frac{DT}{Dt} + \rho\left[\hat{V} - T\left(\frac{\partial \hat{V}}{\partial T}\right)_p\right]\frac{Dp}{Dt}$$

$$= \rho C_p \frac{DT}{Dt} + \left[1 - T\left(\frac{\partial\left(\frac{1}{\rho}\right)}{\partial T}\right)_p\right]\frac{Dp}{Dt}$$

$$= \rho C_p \frac{DT}{Dt} + \left[1 - \left(\frac{\partial \ln\rho}{\partial \ln T}\right)_p\right]\frac{Dp}{Dt} \tag{4.2-16}$$

Substituting Eq. 4.2-16 in Eq. 4.2-14 yields

$$\rho C_p \frac{DT}{Dt} + \left[1 - \left(\frac{\partial \ln \rho}{\partial \ln T}\right)_p\right] \frac{Dp}{Dt} - \frac{Dp}{Dt} + \frac{p}{\rho}\frac{D\rho}{Dt}$$

With the cancellation of equal terms, $\frac{Dp}{Dt}$, in the above equation, we get

$$\rho C_p \frac{DT}{Dt} + \left(\frac{\partial \ln \rho}{\partial \ln T}\right)_p \frac{Dp}{Dt} + \frac{p}{\rho}\frac{D\rho}{Dt} \tag{4.2-17}$$

From the equation of continuity, Eq. 1.4.3-8, we can write

$$-\left(\frac{1}{\rho}\right)\frac{D\rho}{Dt} = (\vec{\nabla} \,.\, \vec{v})$$

Thus, Eq. 4.2-17 can be written as

$$\rho C_p \frac{DT}{Dt} + \left(\frac{\partial \ln \rho}{\partial \ln T}\right)_p \frac{Dp}{Dt} - p(\vec{\nabla} \,.\, \vec{v}) \tag{4.2-18}$$

which is the LHS of Eq. 4.2-13. Putting the terms back into the equation, we get

$$\rho C_p \frac{DT}{Dt} + \left(\frac{\partial \ln \rho}{\partial \ln T}\right)_p \frac{Dp}{Dt} - p(\vec{\nabla} \,.\, \vec{v}) = -(\vec{\nabla} \,.\, \vec{q}) - p(\vec{\nabla} \,.\, \vec{v}) - (\tilde{\tau} : \vec{\nabla}\vec{v}) + \dot{Q}_{\text{other}} - \dot{W}_{\text{other}}$$

Since the third term on the LHS and the second term on the RHS are the same, we can write

$$\rho C_p \frac{DT}{Dt} = -(\vec{\nabla} \,.\, \vec{q}) - (\tilde{\tau} : \vec{\nabla}\vec{v}) - \left(\frac{\partial \ln \rho}{\partial \ln T}\right)_p \frac{Dp}{Dt} + \dot{Q}_{\text{other}} - \dot{W}_{\text{other}} \tag{4.2-19}$$

The above equation is the thermal energy equation in terms of C_p.

4.2.1 Temperature Profile in a Tissue

Let us consider the temperature profiles and the maximum temperature attained in a tissue at steady state – heat is generated due to metabolism. Let us assume that the tissue is a cylinder of radius R, the thermal conductivity is k, and there is uniform and constant heat generation, $\dot{Q}_m$. Let us also assume that the conditions in the body are such that the surface of each tissue is kept at a constant temperature, T_s, and that there is no heat flux along the tissue length. Besides which, let us also assume that no other work is done by the tissue.

Using Eq. B2 (cylindrical coordinates) from Table 4.2-1, in which we can cancel the irrelevant terms

$$\rho C_V\left(\overset{0,\ \text{SS}}{\cancel{\frac{\partial T}{\partial t}}}+\overset{v_r=0}{\cancel{v_r}}\frac{\partial T}{\partial r}+\overset{v_\theta=0}{\cancel{\frac{v_\theta}{r}}}\frac{\partial T}{\partial \theta}+\overset{v_z=0}{\cancel{v_z}}\frac{\partial T}{\partial z}\right)$$

$$=k\left[\frac{1}{r}\frac{\partial}{\partial r}\left(r\frac{\partial T}{\partial r}\right)+\overset{T\neq f(\theta)}{\cancel{\frac{1}{r^2}\frac{\partial^2 T}{\partial \theta^2}}}+\overset{T\neq f(z)}{\cancel{\frac{\partial^2 T}{\partial z^2}}}\right]+\overset{\text{All the velocities are zero}}{\cancel{2\mu\left\{\left(\frac{\partial v_r}{\partial r}\right)^2+\left[\frac{1}{r}\left(\frac{\partial v_\theta}{\partial \theta}+v_r\right)\right]^2+\left(\frac{\partial v_z}{\partial z}\right)^2\right\}}}$$

$$+\overset{\text{All the velocities are zero}}{\cancel{\mu\left\{\left(\frac{\partial v_\theta}{\partial z}+\frac{1}{r}\frac{\partial v_z}{\partial \theta}\right)^2+\left(\frac{\partial v_z}{\partial r}+\frac{\partial v_r}{\partial z}\right)^2+\left[\frac{1}{r}\frac{\partial v_r}{\partial \theta}+r\frac{\partial}{\partial r}\left(\frac{v_\theta}{r}\right)\right]^2\right\}}}+\dot{Q}_{\text{other}}-\underset{\text{No work}}{\cancel{\dot{W}_{\text{other}}}} \tag{4.2.1-1}$$

If we take $\dot{Q}_{\text{other}}-\dot{Q}_m=$ metabolic heat rate, then

$$-\frac{k}{r}\frac{d}{dr}\left(r\frac{dT}{dr}\right)=\dot{Q}_m \tag{4.2.1-2}$$

The boundary conditions are

BC 1: At $r = 0$, T = finite or $\dfrac{dT}{dr} = 0$ (4.2.1-3)

BC 2: At $r = R$, $T = T_s$ (4.2.1-4)

Integrating once with BC 1, we get

$$\frac{dT}{dr}=-\frac{\dot{Q}_m}{2k}r$$

Integrating again with BC 2, we get

$$T=T_s+\frac{\dot{Q}_m R^2}{4k}\left[1-\left(\frac{r}{R}\right)^2\right] \tag{4.2.1-5}$$

Now, let us attempt to express the results in a more general fashion. If we non-dimensionalise the variables

$$\theta=\frac{T-T_s}{\dfrac{\dot{Q}_m R^2}{4k}}$$

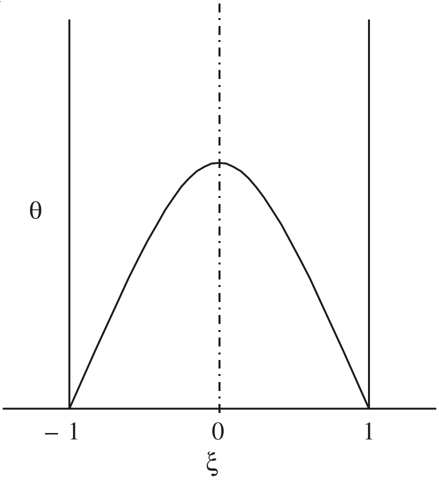


Fig. 4.2.1-1 Non-dimensionalised temperature profile in the tissue

and

$$\xi = \frac{r}{R}$$

the solution becomes

$$\theta = 1 - \xi^2 \qquad (4.2.1\text{-}6)$$

A plot of the variation of θ along the tissue length is shown in Fig. 4.2.1-1.

The rate of heat dissipation at the cylindrical surface, for the tissue length, L is

$$\text{Area} \times \text{Flux} = 2\pi RL \times q_r|_{r=R} \qquad (4.2.1\text{-}7)$$

$$= 2\pi RL\left(-k\frac{dT}{dr}\right)\bigg|_{r=R} = \pi R^2 L\dot{Q}_m \qquad (4.2.1\text{-}8)$$

From Eq. 4.2.1-5, we can say that $T_{\max}$ occurs when $r = 0$.

Thus

$$T_{\max} = T_s + \frac{\dot{Q}_m R^2}{4k}$$

For $R = 1$ cm, $\dot{Q}_m = 5$ cal cm^{-3} h^{-1}, $k = 10^{-3}$ cal (cm.s.°C)$^{-1}$ and $T_s = 37$ °C, we get

$$T_{\max} = 37 + \frac{5 \times 1^2}{(4 \times 10^{-3})3600} = 37.3\ °\text{C}$$

The temperature at the centre of the tissue could be 0.3 °C higher than at the surface.

4.2.2 Unsteady State Heat Conduction

Let us discuss unsteady state heat conduction through an example.

Example 4.2.2-1

In a microanalysis system, to determine an analyte, the sample is first sprayed as 10 μl spherical droplets into a heating zone. The droplets need to be heated to 60 °C to complete a reaction that is a necessary step for the analysis. Assuming that the properties of a sample drop are the same as that of water (since the sample is predominantly aqueous), estimate the time needed to reach the steady state temperature in the droplet.

Since we are dealing with a sphere, it is most convenient to use spherical coordinates. Thus, from Eq. C2 of Table 4.2-1, we get, after cancelling the irrelevant terms

$$\frac{\partial T}{\partial t} = \left(\frac{k}{\rho C_V}\right)\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial T}{\partial r}\right) \tag{4.2.2-1}$$

Let us define $\left(\frac{k}{\rho C_V}\right) \equiv \sigma$.

We can consider the drop surface temperature being raised to 60 °C (T_s) at the start of the cycle, $t = 0$.

Thus

$$\text{IC: For } 0 < r < R, \quad t \le 0, \quad T = T_0 \tag{4.2.2-2}$$

$$\text{BC 1: For } r = 0, \quad t \ge 0, \quad \frac{\partial T}{\partial r} = 0 \tag{4.2.2-3}$$

$$\text{BC 2: For } r = R, \quad t \ge 0, \quad T = T_s \tag{4.2.2-4}$$

If we use non-dimensional variables defined as

$$\eta = \frac{r}{R}$$

$$\theta = \frac{T - T_0}{T_s - T_0}$$

and

$$\tau = \frac{\sigma t}{R^2}$$

the DE, the IC and the BCs respectively, become

$$\frac{\partial \theta}{\partial \tau} = \frac{1}{\eta^2}\frac{\partial}{\partial \eta}\left(\eta^2 \frac{\partial \theta}{\partial \eta}\right) \tag{4.2.2-5}$$

$$0 < \eta < 1, \qquad \tau \le 0, \qquad \theta = 0 \tag{4.2.2-6}$$

$$\eta = 0, \qquad \tau \ge 0, \qquad \frac{\partial \theta}{\partial r} = 0 \tag{4.2.2-7}$$

$$\eta = 1, \qquad \tau > 0, \qquad \theta = 1 \tag{4.2.2-8}$$

We cannot apply separation of variables to get the solution of the above differential equation because for that the BCs need to be homogenous. Thus, let us use the following transformation:

$$\theta'(\eta, \tau) = 1 - \theta(\eta, \tau) \tag{4.2.2-9}$$

The transformed problem is

$$\frac{\partial \theta'}{\partial \tau} = \frac{1}{\eta^2}\frac{\partial}{\partial \eta}\left(\eta^2 \frac{\partial \theta'}{\partial \eta}\right) \tag{4.2.2-10}$$

$$0 < \eta < 1, \qquad \tau \le 0, \qquad \theta' = 1 \tag{4.2.2-11}$$

$$\eta = 0, \qquad \tau \ge 0, \qquad \frac{\partial \theta'}{\partial r} = 0 \tag{4.2.2-12}$$

$$\eta = 1, \qquad \tau > 0, \qquad \theta' = 0 \tag{4.2.2-13}$$

If we define $f = \theta'\eta$, then Eq. 4.2.2-10 becomes

$$\frac{\partial f}{\partial \tau} = \frac{\partial^2 f}{\partial \eta^2} \tag{4.2.2-14}$$

The solution is

$$\theta' = \left[\frac{A}{\eta}\sin(\lambda\eta) + \frac{B}{\eta}\cos(\lambda\eta)\right]\exp(-\lambda^2\tau) \tag{4.2.2-15}$$

and

$$\theta = 1 + \sum_{n=1}^{\infty} \frac{2(-1)^n}{\eta(n\pi)}\sin(n\pi\eta)\exp(-n^2\pi^2\tau) \tag{4.2.2-16}$$

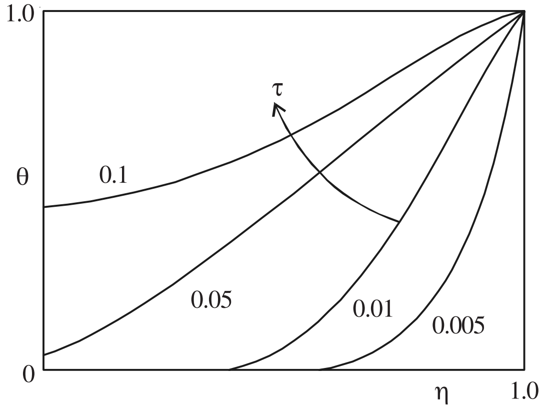
The variation of the non-dimensional temperature with non-dimensional distance at various values of non-dimensional time is given in Fig. 4.2.2-1.

The τ needed for the $T|_{r=0}$ to reach 99 % of T_s is about 0.5. Thus, τ for steady state condition = 0.5, or

$$\frac{t\sigma}{R^2} = 0.5$$

$$t|_{ss} = \frac{0.5R^2}{\sigma}$$

Fig. 4.2.2-1 Non-dimensionalised profile in the drop



Now for the spherical drop

$$R = \left(\frac{3V}{4\pi}\right)^{\frac{1}{3}} = \left(\frac{3\times 0.01}{4\pi}\right)^{\frac{1}{3}} = 0.134 \text{ cm} = 1.34 \times 10^{-3} \text{ m}$$

$\sigma_{\text{water}} \sim 1.5 \times 10^{-7}$ m^2 s^{-1}. Thus

$$t|_{ss} = \frac{0.5(1.34\times 10^{-3})^2}{(1.5\times 10^{-7}\,\text{m}^2\text{s}^{-1})} \cong 6 \text{ s}$$

Exercises

1. Is thermal energy conserved? If not, why do we focus on thermal energy in this chapter?

2. Show that

$$(\vec{v}\cdot[\vec{\nabla}\cdot\tilde{\tau}]) - (\vec{\nabla}\cdot[\tilde{\tau}\cdot\vec{v}]) = -(\tilde{\tau}:\vec{\nabla}\vec{v})$$

3. In forced convection, what is the driving force for the heat flux?

4. I had the privilege of contributing significantly to the setup of the new Department of Biotechnology at IIT Madras as the head in its formative years, 2005-2008. In 2006, when we moved into our new department building, we had a difficult time cooling the conference room that was located on the top floor with the available a/c capacity. One of the solutions suggested by a consultant was to attach thermocol sheets to the ceiling surface inside the room. If we were aiming at a temperature reduction of about 5 °C from the room ceiling inner surface temperature of 42 °C so that the available a/c

system could handle the load, would a thermocol layer of 0.75 m thickness have served our purpose, assuming that the walls and double-glazed windows are insulating, i.e. no heat transfer occurs through them? The thermal conductivity of thermocol is 0.03 W (m K)$^{-1}$. The room dimensions are 12 m × 10 m × 3 m. Based on the estimates of solar energy striking the ceiling top surface, and that absorbed by it, as well as that reflected from it, the energy rate into the room from the inner ceiling surface is 600 W m^{-2}.

5. Humans maintain their body temperature at 37 °C through metabolic heat generation. Consider a pleasant day when the ambient temperature is 25 °C. Under still conditions (no breeze, etc.), estimate and compare the contribution of heat loss rate from the human body by conduction to that by radiation. The radiative heat flux (q_r), as may be known, is given by Stefan-Boltzmann's law, with T in K, as

$$q_r = \sigma \in \left(T_{\text{body}}^4 - T_{\text{surr}}^4\right)$$

   Take the area of the human body to be 2 m^2, thermal conductivity of air = 5.7×10^{-5} cal (cm °C)$^{-1}$, σ, the Stefan-Boltzmann constant = 5.67×10^{-8} W m^{-2} K^{-4}, and ε, emissivity of the human body = 0.97. Assume that the temperature reaches the ambient air temperature at 5 cm distance from the human skin.

6. The average thickness of the earth's crust, the top-most layer is 25 km out of a total of about 6300 km radius. The temperature just beneath the crust is 400°C, and the average atmospheric temperature is 25 °C. If the thermal conductivity of the crust is 2.5 W m^{-1} K^{-1}, find the thermal energy lost by the earth.

7. Significant damage of the skin cells due to heat ('burn') results when the temperature on the cell/tissue surface reaches say 85 °C. When a person comes into contact with the hot surface of a hot plate (at 250 °C) in the lab, and takes say 0.3 s to react and move away, estimate the depth of the burn caused. The physical properties of skin are: specific gravity: 1.2, conductivity: 0.21 W (m K)$^{-1}$, specific heat capacity at constant pressure: 3.6 KJ (kg °C)$^{-1}$.

8. In the first of the Harry Potter books, Stone, forgetful Neville's grandmother sent him a Remembrall. This is a spherical ball of radius 3 cm, which glows red whenever he forgets something. To shoot those scenes in the movie, a battery powered light that glows on a cue was probably used. Assume that 2 amps, 1.5 V is used as the power source, and the surface of the temperature is 300 K. The glow of the light source dissipates heat radially outward in the still air inside the Remembrall. Develop an expression for the temperature profile as a function of radial distance inside the Remembrall.

9. People who live in the colder regions of our country, where the temperatures can dip to a few degrees below the water freezing point, wear bulky coats.

These coats are usually more effective than thick woollen sweaters alone, because they consist of multiple layers of materials with low heat conductivity, which maximise heat retention by the body. Usually there are three layers in such coats, two layers with feathers with a foam layer between them, in a 2:1:3 thickness ratio with the foam layer thickness being 1 cm. If the thermal conductivities of the feather and the foam layers are 6×10^{-5} and 1.3×10^{-4} W $(\mathrm{m\ K})^{-1}$ respectively, evaluate whether the coat will be able to maintain the body temperature of 37 °C when the outside temperature is 2 °C, under no breeze conditions.

10. In fishes, typically, when cold blood passes through muscles, the blood picks up the heat generated by the muscles and, thus, heat is not lost to the surroundings. A muscle of interest in the fish can be assumed to be a cylinder of length 10 cm, and radius, 3 cm. If the temperature at the core of the muscle is 30 °C, and drops to 28 °C at its surface, where the blood vessels pick up the heat from the muscle, find the rate of metabolic heat generation in the muscle. The thermal conductivity of the muscle can be taken to be 0.56 W m^{-1} K^{-1}.

Some of the exercise problems given above were suggested/formulated by S. Kousik, Sagar Laygude, Utsav Saxena (5), P. Raghavendran, P. Vivek, K. Ramasamy, M. Ashok (6, 10), Shruthy Suresh and Purnima Padmanabhan (8, 9).

Fully Open-ended Exercise

Estimate the heat rate by conduction while preparing a dosa. This problem was formulated by Indushri Gokak, for her CFA exercise on the heat transfer aspects that are relevant when a dosa is prepared (CFA stands for choose-focus-analyse exercise; see end of Chapter 1 for a relevant reference). Indushri's report can be found as a link from www.biotech.iitm.ac.in/GK_research.

Reference

Bird RB, Stewart WE, Lightfoot EN (2002) Transport phenomena. Second Edition. John Wiley, Singapore

Part IV
Charge Conservation

Chapter 5
Charge Flux

Many fundamental biological entities carry charges. For example, from a basic biochemistry course, we know that amino acids have a charge associated with them and that the charge is pH dependent. Consequently, polymers of amino acids, namely proteins, also carry charges and the net charge carried by a protein is pH dependent. The genetically important molecule, deoxyribonucleic acid (DNA), too, is charged. The third major class of bio molecules, lipids, can also have charges associated with them. Since lipids and proteins constitute cell membranes, the surface of cells have a net charge. The charge is usually net negative.

It is only because of charges and their dynamics that we are able to sense our environment through sight, smell, taste, touch and hearing. The dynamics of charges are also essential for the functioning of our nervous system, our brain and our heart.

Since charge is a fundamental physical quantity that is conserved, a better understanding of the fundamental relationships related to electrical charges and the consequent or parallel aspect, magnetism, can significantly equip the manipulator of biology. The aspect of charge conservation is inherent in the basic tenets of electromagnetism and Maxwell's equations, and thus, we need to study them first.

To understand the effects of electric and magnetic fields, the space between interacting charges can be considered to be influenced by the charges, as imagined first by Faraday. The forces between (say two) like charges are transferred from one charge to the other through the space in which they are located. Thus, electric and magnetic 'fields' exist at a point in space even in the absence of charges at that particular point.

To be able to visualise the electromagnetic field better, let us first consider the effect of this field on a charged particle, and the force experienced by the particle.

G.K. Suraishkumar, *Continuum Analysis of Biological Systems*, Biosystems & Biorobotics 5,
DOI: 10.1007/978-3-642-54468-2_5,

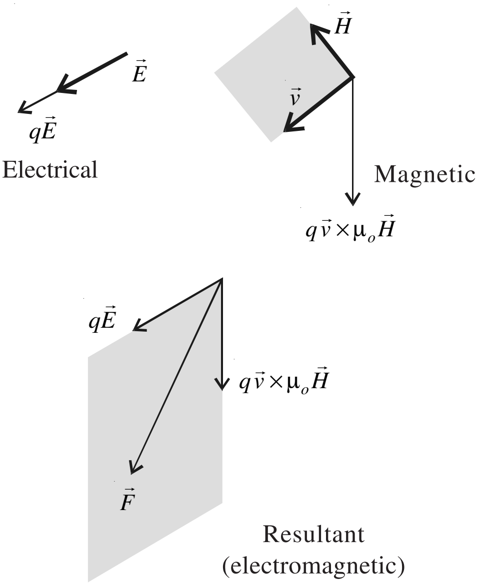


Fig. 5.1-1 The vectorial representation of the combined effects of an electrical and a magnetic field – the forces that result from them

5.1 Lorentz Force Law

The force $\vec{F}$ experienced by a test charge q that moves at a velocity $\vec{v}$ in such a field is given by the Lorentz force law

$$\vec{F} = q(\vec{E} + \vec{v}\times\mu_o\vec{H}) \qquad (5.1\text{-}1)$$

where $\vec{E}$ is the electric field density, $\vec{H}$ is the magnetic field intensity, $\mu_o\vec{H}$ is the magnetic flux density and μ_o is the permeability of free space = $4\pi \times 10^{-7}$ Henry m^{-1}, Henry = Volts (amp)$^{-1}$.

Vectorically it can be represented as shown in Fig. 5.1-1.

5.2 Charge Density and Flux

Useful quantities for further formulations are *charge density* and *charge flux*. Charge flux is also called *current density*.

If we consider a small volume, ΔV with a net charge within, the charge density, ρ, is defined as

$$\rho \equiv \frac{\text{Net charge in } \Delta V}{\Delta V}\ \text{coulomb m}^{-3} \qquad (5.2\text{-}1)$$

ΔV is usually chosen to be much smaller compared to the system dimensions, but large enough to contain many charges to ensure continuum conditions.

Current is charge transport and is a measure of the rate of change of charge with time. If a charge density ρ moves with a velocity $\vec{v}$, the charge flux $\vec{I}\,'$ is denoted as

$$\vec{I}\,' = \rho\vec{v} \text{ in coulomb m}^{-2}\text{s}^{-1} \tag{5.2-2}$$

5.3 Maxwell's Relations

The Lorentz force law (Section 5.1) expresses the effect of electromagnetic fields on a charge. The effects of the charge (moving or stationary), and its relationship to the fields created by it are described by Maxwell's equations. The aspect of charge conservation (total charge is a constant) is implicit in these equations, and is obvious in Maxwell's first relation.

5.3.1 How is the Electric Field Related to its Source?

The net charge enclosed by an arbitrary volume V which is enclosed by a surface S is given by Maxwell's (first) relation

$$\oint_S \epsilon_o \vec{E}.d\vec{A} = \int_V \rho dV \tag{5.3.1-1}$$

where ϵ_o is permittivity of free space = 8.854 × 10^{-12} Farad m^{-1}. Further, note that $\int_V \rho dV = Q$.

In other words, the net charge enclosed in a volume V, enclosed by a surface S is related to the net electric flux through that surface. Equation 5.3.1-1 is also called Gauss' law.

5.3.2 How is the Magnetic Field Intensity Related to its Source, the Charge Flux?

Maxwell's (second) relation shows how the magnetic field intensity is related to its source, as follows

$$\oint_C \vec{H}.d\vec{S} = \int_S \vec{I}\,'.d\vec{A} + \frac{d}{dt}\int_S \epsilon_o \vec{E}.d\vec{A} \tag{5.3.2-1}$$

This is also known as Ampere's integral law.

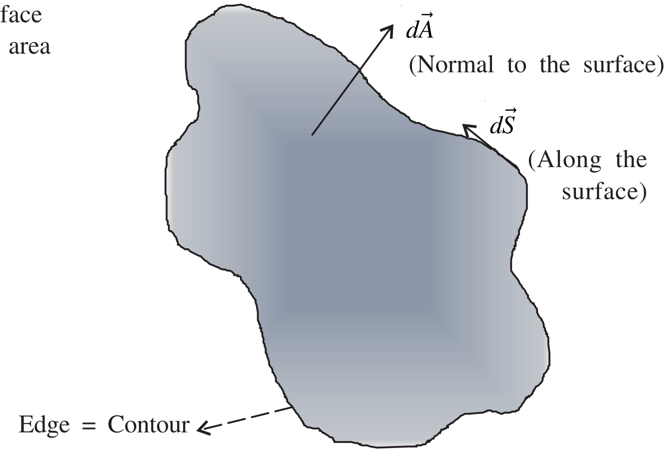


Fig. 5.3.2-1 A surface with two different area vectors

The LHS of Eq. 5.3.2-1 indicates a contour integral. A surface *S* having a contour *C* is given in Fig. 5.3.2-1. The differential elements, $d\vec{S}$ and $d\vec{A}$, are also indicated: $d\vec{S}$ is along the surface, whereas, $d\vec{A}$ is normal to the surface.

In other words, the line integral (circulation) of the magnetic field intensity $\vec{H}$ around a closed contour is equal to the sum of the net current passing through the surface spanning the contour and the time rate of change of the net displacement flux density (displacement current) through the surface.

Alternatively, Eq. 5.3.2-1 can be written as

$$\oint \vec{H}.d\vec{S} = I + \epsilon_o \frac{d\phi_E}{dt} \tag{5.3.2-2}$$

where ϕ_E is electric 'flux' (historically called flux – we use quotes here to avoid confusion in our context) and *I* is current.

In other words, an electric current and a time-variant electric 'flux' produce a magnetic field.

5.3.3 How are Electric Field and Magnetic Flux Related?

The relationship between an electric field and the magnetic flux is given by Maxwell's (third) relationship

$$\oint_C \vec{E}.d\vec{S} = -\frac{d}{dt}\int_S \mu_o \vec{H}.d\vec{A} \tag{5.3.3-1}$$

This is also known as Faraday's integral law.

In terms of the magnetic 'flux' (the term flux here is again, historical), ϕ_B, this can also be written as

$$\oint \vec{E}.d\vec{S} = -\frac{d\phi_B}{dt} \tag{5.3.3-2}$$

5.3.4 A Comment on the Net Magnetic Flux Out of Any Region

The net magnetic flux out of any region enclosed by a surface is zero. This is Maxwell's (fourth) relationship and is also known as Gauss' integral law.

Mathematically, it can be expressed as

$$\oint_S \mu_o \vec{H}.d\vec{A} = 0 \tag{5.3.4-1}$$

5.4 An Expression for Charge Conservation

It is useful to obtain a relationship for charge conservation in terms of charge and charge flux. The principle of charge conservation can be stated as the net charge flowing out of the system, given by the rate of charge leaving through the surface boundaries of the system, $\int_S \vec{I}'.d\vec{A}$, is equal to the rate of decrease of charge within the system, $-\frac{d}{dt}\int_S \epsilon_o \vec{E}.d\vec{A}$. In other words, when there is no input, or generation, or consumption of charge, the rate of output must equal the rate of (negative) accumulation in the system. In the form of an equation, the above principle can be written as

$$\int_S \vec{I}'.d\vec{A} + \frac{d}{dt}\int_S \epsilon_o \vec{E}.d\vec{A} = 0 \tag{5.4-1}$$

From Maxwell's (first) relationship, Eq. 5.3.1-1, we can replace the second term on the LHS of Eq. 5.4-1 as

$$\int_S \vec{I}'.d\vec{A} + \frac{d}{dt}\int_V \rho dV = 0 \tag{5.4-2}$$

5.5 Maxwell's Equations in Differential Form

$$\vec{\nabla}.\epsilon_o\vec{E} = \rho \tag{5.5-1}$$

$$\vec{\nabla}\times\vec{H} = \vec{I}' + \frac{d}{dt}\epsilon_o\vec{E} \tag{5.5-2}$$

$$\vec{\nabla}\times\vec{E} = -\frac{d}{dt}\mu_o\vec{H} \tag{5.5-3}$$

$$\vec{\nabla}.\mu_o\vec{H} = 0 \tag{5.5-4}$$

And the equation of charge conservation in differential form is

$$\vec{\nabla}.\vec{I}' + \frac{d\rho}{dt} = 0 \quad \text{or} \quad \vec{\nabla}.\vec{I}' + \frac{\partial\rho}{\partial t} = 0 \tag{5.5-5}$$

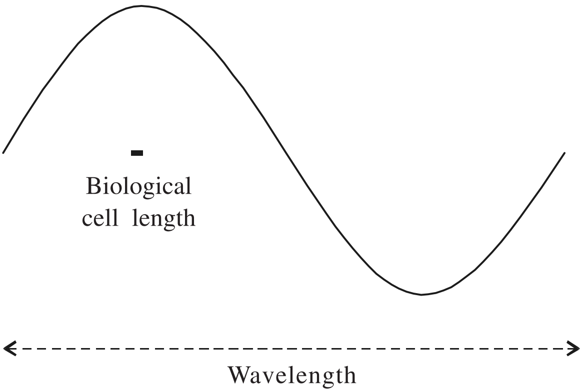
In the above presentation of Maxwell's equations, we had implicitly assumed that there was no medium present, i.e. the processes were assumed to take place in free space. Thus, the electrical properties of free space, ϵ_o and μ_o were used. However, most biological processes take place in a medium, typically a liquid because under physiological conditions, cells are in an appropriate liquid. When electromagnetic fields interact with the medium (or any material), the fields induce effects such as polarisation and magnetisation in the medium.

Polarisation arises because of the nature of the biological media – they contain molecules with positive and negative charge centres that are separated by a distance, or in other words, they have permanent dipole moments. Water, which is found in almost all biological systems, has a permanent dipole moment, and so do biomolecules. The distribution of dipoles is usually random in a biological material, but, when an electric field is applied, there is an alignment, at least partial, of the dipoles with the field. Such an alignment changes the electrical behaviour of the media and is called polarisation. In a similar fashion, magnetisation arises due to the interaction of the magnetic dipole moments with the magnetic field. Electrical and magnetic effects are coupled.

The earlier mentioned Maxwell's equations need to be improved when written for biological systems in a media, or under non-free space conditions. For example, in the presence of an electric field, there could be free and polarised charges in the medium. Let us represent the charge densities as ρ_{fc} (due to free charges) and ρ_{pc} (due to polarised charges). Thus, the Gauss' law for this system becomes

$$\vec{\nabla}.\epsilon\vec{E} = \rho_{fc} + \rho_{pc}$$

Fig. 5.5-1 Length scale of a typical cell compared with the length scale of an electromagnetic wave



In fact, the form of Maxwell's equations for *isotropic* media (uniform media, or media in which its properties remain the same with space), remain the same except for the replacement of the free space permittivity, ϵ_o, by the medium permittivity, ϵ. Interestingly, the permeability of most biological materials such as cells and tissues, can be approximated very well to μ_o.

Further, the wavelengths of the electromagnetic spectrum of relevance to biological systems range from about 10^{12} m (low frequency waves or 'infralow' frequency waves) to about 10^{-4} m (microwaves or 'superhigh' frequency waves), whereas cells and many biologically important dimensions such as microchannels, etc., are about 10^{-6} m. A rough representation is given in Fig. 5.5-1. Therefore, the time of interaction of the wave with the cell, which is two orders of magnitude less in size compared to its wavelength, is two orders of magnitude less compared to the time the wave takes to complete its variations with time. Comparing this situation with the characteristic times of the various processes described in Chapter 2, when we discussed the pseudo-steady state, we can say that the cell interaction times are at pseudo-steady state compared to the wave times. In other words, any fluctuation in the times associated with the cell interaction will not be noticeable at the scales of time associated with the wave.

Thus, for most applications in biology, the electro-quasi-state (EQS) and the magneto-quasi-state (MQS) approximations that hold good for electromagnetic formulations at low enough frequencies, work well. The steady-state approximations essentially set the time derivatives in Maxwell's equations to zero. The approximate Maxwell's equations in differential form are

$$\vec{\nabla}.\epsilon\vec{E} = \rho \tag{5.5-6}$$

$$\vec{\nabla}\times\vec{H} = \vec{I}' \tag{5.5-7}$$

$$\vec{\nabla}\times\vec{E} = 0 \tag{5.5-8}$$

$$\vec{\nabla}.\mu\vec{H} = 0 \tag{5.5-9}$$

Also

$$\vec{E} = -\vec{\nabla}\mathbf{V} \tag{5.5-10}$$

where **V** is the potential.

Therefore

$$\vec{\nabla}.\epsilon\,\vec{E} = \vec{\nabla}.(-\epsilon\vec{\nabla}\mathbf{V})$$

By substituting this in Eq. 5.5-6, we get

$$\vec{\nabla}.(-\epsilon\vec{\nabla}\mathbf{V}) = \rho$$

Therefore

$$\nabla^2\mathbf{V} = -\frac{\rho}{\epsilon} \tag{5.5-11}$$

which is known as the Poisson equation. In the region where no charges are present ($\rho = 0$), the RHS of the Poisson equation becomes zero and we get

$$\nabla^2\mathbf{V} = 0 \tag{5.5-12}$$

which is known as the Laplace equation. These equations are useful in the analysis of biological systems, e.g. certain marine organisms such as the electric eel can be considered to be an electric dipole that satisfies the Laplace equation.

5.5.1 Application of Maxwell's Equations to Get Useful Relationships

Maxwell's equations are a complete description of the electromagnetic phenomena, and hence we began our discussion with them. While dealing with continuous systems, a manipulator of biology will never fall short, if Maxwell's equations are involved. However, they are not always easy to use in certain situations, and special case derivations of the equation along with constitutive equations such as Ohm's law, that relates current and voltage when certain types of materials are considered, are more useful.

In this section, we will demonstrate how Maxwell's equation can be used to derive the capacitor equation. It can be recalled that the biological membrane consists of lipids, proteins and carbohydrates. The lipid molecule consists of a hydrophilic, charged head and a hydrophobic tail. When the

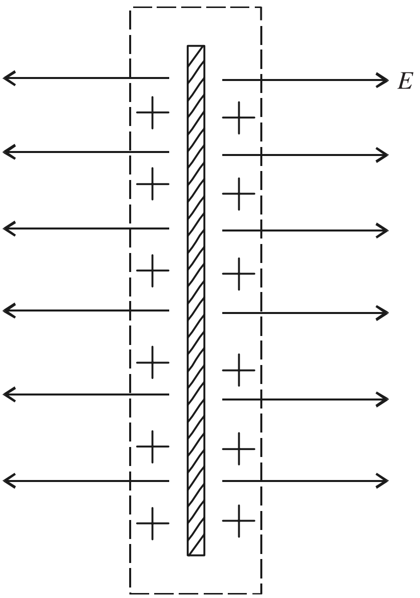


Fig. 5.5.1-1 The electric field due to a charged plate, charged on both surfaces

lipid bilayer assembles together, energy considerations dictate that the hydrophobic tails be close together and the hydrophilic parts be at opposite ends of the bilayer membrane cross-section. The charged hydrophilic parts face the internal part of the cell on one end and the cell surroundings on the other end. Since the internal part of the cell and the cell surroundings are usually made up of conducting solutions, the lipid bilayer separates two conducting solutions by a thin insulating (hydrophilic part) layer. Thus, the very nature of the bilayer and its surroundings makes it an electrical capacitor.

Let us consider a flat surface of area A of uniform charge density ρ and uniform surface charge density ρ′ as shown in Fig. 5.5.1-1. Let us consider a cuboidal control volume around it, which is shown in the figure as a rectangle around the flat surface.

To draw the electric flux lines for the charged plate, the following principle is used: an electric flux line always starts in a positive charge and ends in a negative charge. If the charge is a point charge, Fig. 5.5.1-2 shows the flux lines.

Getting back to the flat surface, the charge contained in the control volume is $\rho'(2A)$ since there are two surfaces, each of area A.

Let us now consider a capacitor of plate area A as shown in Fig. 5.5.1-3. From Gauss' law (Maxwell's relation)

$$\oint_S \vec{E}.d\vec{A} = \frac{Q}{\epsilon_o}$$

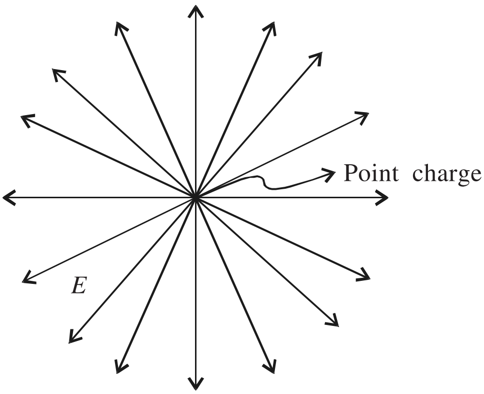


Fig. 5.5.1-2 The electric field *E* due to a point charge

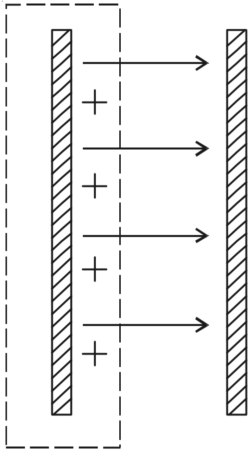


Fig. 5.5.1-3 A typical parallel plate capacitor

In this case, since there are two surfaces each of area *A*

$$\vec{E}(2A) = \frac{\rho'(2A)}{\epsilon_o} \tag{5.5.1-1}$$

Therefore

$$\vec{E} = \frac{\rho'}{\epsilon_o} \tag{5.5.1-2}$$

The integral of the electric field with respect to displacement gives the potential difference

$$\Delta \mathbf{V} = \int \vec{E}.d\vec{l} \tag{5.5.1-3}$$

In this case, the integral yields

$$\Delta \mathbf{V} = \frac{\rho' d}{\epsilon_o} \tag{5.5.1-4}$$

where d is the distance between the capacitor plates.

Replacing ρ' by Q/A, we get

$$\Delta \mathbf{V} = \frac{Qd}{A\epsilon_o} \tag{5.5.1-5}$$

The capacitance C, defined as $\dfrac{Q}{\Delta V}$ is, therefore

$$C = \frac{A\epsilon_o}{d} \tag{5.5.1-6}$$

which is a known relationship of a parallel plate capacitor.

5.5.2 Electroencephalogram (EEG)

An electroencephalogram is obtained by recording the voltage on the skull surface. The voltage is caused by currents that are generated in the brain. Although the natures of the currents in the brain are interesting by themselves, for initial purposes, we can consider the brain to be a charge of a certain density enclosed in a volume (skull). In fact, it can be considered as a non-homogenous, finite volume of charges.

Starting from the fundamental equations presented in the earlier sections, it has been shown (Malmivuo and Plonsey 1995) that for a non-homogenous, finite volume conductor, the following equation holds:

$$4\pi k_e \mathbf{V} = \int_V \vec{I}\,'\cdot\nabla\left(\frac{1}{r}\right)dV + \sum_j \int_S (k_{e,2j} - k_{e,1j})\mathbf{V}\nabla\left(\frac{1}{r}\right)\cdot d\vec{S} \tag{5.5.2-1}$$

where k_{e2} and k_{e1} are conductances at the limiting differential surfaces of the inhomogenous conductor divided into differential regions.

The nature of the EEG gives an idea of the brain activity. Some limiting cases are presented in Fig. 5.5.2-1.

5.6 Constitutive Equation

Let us recall that Fick's first law, which provided a relationship between diffusive flux and concentration gradient, is valid for a class of materials,

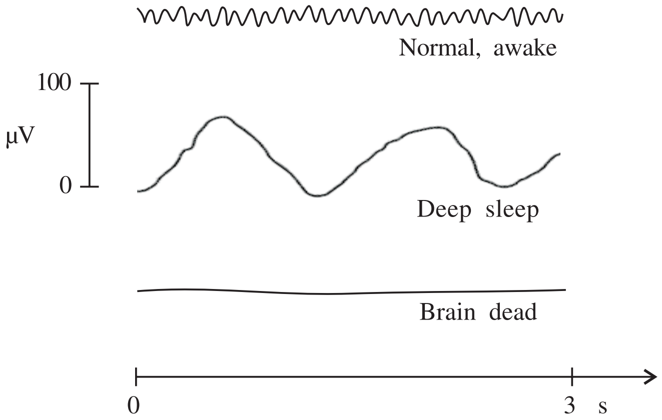


Fig. 5.5.2-1 EEG traces under some limiting cases

and is thus, a constitutive equation. Similar to that relationship, for certain materials, the charge flux is proportional to the potential gradient, i.e.

$$\vec{I}\,' = -k_e \vec{\nabla}\mathbf{V} = k_e \vec{E} \tag{5.6-1}$$

where k_e is the electrical conductivity of the medium (typical unit: Siemens cm^{-1}).

This is a constitutive equation, which is valid for a class of materials, and is known as the Ohm's law.

5.7 Ions in Solutions

Let us now consider charged species (ions) in solution. Since most cells are in an aqueous environment and their contents too are fluid, this aspect is of great importance in biological systems.

5.7.1 Electro Neutrality

Although oppositely charged ions are present in a solution, the strong forces of attraction between them results in electro neutrality (no net charge). Thus, an electrolytic solution does not set up an electric field although it contains charges.

5.7.2 Charge Relaxation Time

Let us consider an uniform initial charge density, ρ_o in the medium (say, which is homogenous, isotropic, conducting, dielectric with no movement of any charge). If there is no supply (source) of free charge, the initial charge will decay to zero because the medium is conducting. To estimate the time at which the decay to zero charge (charge relaxation) occurs, let us consider the following:

The charge flux (current density), according to Ohm's law is

$$\vec{I}\,' = k_e \vec{E} \tag{5.7.2-1}$$

where $\vec{E} = -\vec{\nabla}\mathbf{V}$.

Since we are considering the electrolytic solution to be a homogenous conductor (k_e is constant)

$$\vec{\nabla}.\vec{I}\,' = k_e \vec{\nabla}.\vec{E} \tag{5.7.2-2}$$

From Gauss' law, we know that

$$\vec{\nabla}.\epsilon\vec{E} = \rho \tag{5.7.2-3}$$

where ρ is charge density at any time t.

Therefore, by substituting Eq. 5.7.2-3 into 5.7.2-2, we get

$$\vec{\nabla}.\vec{I}\,' = \frac{k_e}{\epsilon}\rho \tag{5.7.2-4}$$

If we assume that upon application of ρ_o, the increase in charge density in the solution is uniform, we can use Eq. 5.5-5, the charge conservation (charge continuity) equation here, i.e.

$$\vec{\nabla}.\vec{I}\,' = -\frac{\partial\rho}{\partial t} \tag{5.5-5}$$

Substituting the above equation in 5.7.2-4, we get

$$\frac{\partial\rho}{\partial t} + \frac{k_e}{\epsilon}\rho = 0 \tag{5.7.2-5}$$

The solution of the differential equation given in Eq. 5.7.2-5 is

$$\rho = \rho_o \exp\left(\frac{-t}{\tau_r}\right) \tag{5.7.2-6}$$

where $\tau_r = \dfrac{\epsilon}{k_e}$ is the charge relaxation time.

For water with $k_e = 0.01$ S cm^{-1}, $\epsilon = 80\,\epsilon_o = 80 \times 8.85 \times 10^{-12}$ F cm^{-1}, $\tau_r = 0.7$ ns, charges can be relaxed rapidly. Charge relaxation needs to be considered while designing systems in which the biological materials – cells, biomolecules, etc. – interact with electrical fields such as in electrophoresis.

5.7.3 Debye Length

Let us consider a specially made lipid layer with uniform surface charge density stretched on a flat plate at $x = 0$. Let us also consider this lipid layer to be bathed by an electrolytic solution with cations and anions. Mobile ions whose charge is opposite to that of the fixed charge (counter ions) will be attracted near the plate. Thus, near the plate, there is a regime where electro neutrality does not hold – it will be charged with the charge of the counterions. Debye length is the distance of such a regime where electro neutrality does not hold. It can be derived (Weiss 1996) to be

$$\lambda_D = \sqrt{\frac{\epsilon RT}{2Z^2F^2c}} \tag{5.7.3-1}$$

where ϵ is permittivity, Z is charge, F is Faraday's constant and c is concentration of positive or negative ions at 'infinite' distance in the solution where electro neutrality holds.

A typical Debye length in aqueous solution is 10 Å.

Charge carrying biomolecules in a system do not generate an electric field because they are shielded by counter ions. Nevertheless, if an electric field is applied, the double-layer counter ion cloud surrounding the charged biomolecule gets disturbed. Then, the charged biomolecule experiences the presence of the field and moves in response to it.

Many electrically relevant phenomena occur in biological systems due to charge transport across the biological membrane. The biological membrane, simplistically speaking, is made up of a bilayer of lipids and proteins. Some proteins act as ion channels for the transport of charged ions across the membranes; it may be recalled that the charged species cannot permeate through the lipid bilayer at reasonable rates. The dynamics of ion transport across the cell is significantly responsible for the signal transmission in nerves, functioning of heart cells, and the normal functioning of almost all cells. When charge transport occurs across the biological membrane, at least two driving forces are at play, namely the potential difference and the concentration difference. Since we will consider the fluxes when more than one driving force is at play, in the next chapter, there we will look at the details of this fascinating phenomenon.

Exercises

1. Explain how the idea of charge conservation is embedded in Maxwell's equations.

2. Consider a bi-layered micelle. It can be taken as a capacitor consisting of charged species on the surfaces of the outer and inner spheres (lipid heads) with an insulator (lipid tails). What work would be needed to place a charge $+ Q$ on one surface and $- Q$ on the other surface?

3. A careless student performs two experiments, side by side. In the first experiment, (s)he is testing the reaction between blood and a sphere of a new material for a pace-maker in the presence of an electric field of magnitude E. Now (s)he accidently drops a small amount of NaCl in the blood, that would completely ionise to give charges, which (s)he was supposed to add to the second experiment. Develop an expression for the time the student needs to wait after which (s)he can carry out the experiment again, without changing any step.

4. In the scenario given in the previous problem, the student immediately removes the sphere from the first experiment and puts it into the vessel containing blood meant for the second experiment. (S)he observes the effect of an electric field which appears even without switching on the external electric field. Help the student make sense of the observations.

5. Consider a dog whose fur is rubbed with a glass rod, so that both the dog and the glass rod acquire charges. For a first rough approximation, we can assume that the electric field produced by the charges on the dog is spherically symmetric. Let the field be E at a distance r from the centre. Calculate the charge on the glass rod.

Some of the exercise problems given above were suggested/formulated by Uma Maheswari, Namrata Kamat, Kiran, Kemun Khimun, Rashmi Kumari (2–4), G. Shashank, G. Vivek Sathvik, D. Divya Vani and I. Pradeep Kumar (5).

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Part V

Multiple Conservations Simultaneously Applied

Chapter 6
Fluxes Under Simultaneous, Multiple Driving Forces

In the previous chapters, we considered the fluxes of various quantities, mostly conserved quantities under the effect of the corresponding primary driving forces. We can summarise what we learnt in the table given below.

Flux of quantity	Primary driving force	A constitutive equation
Mass (conserved quantity)	Concentration gradient	Fick's I law $J_A^* = -D_{AB}\dfrac{dc_A}{dx}$
Momentum (conserved quantity)	Velocity gradient	Newton's law $\tau_{yx} = -\mu\dfrac{dv_x}{dy}$
Thermal energy (not conserved)	Temperature gradient	Fourier's law $q_x = -k\dfrac{dT}{dx}$
Charge (conserved quantity)	Electrical potential gradient	Ohm's law $I' = -k_e\dfrac{d\mathbf{V}}{dx}$

In most biologically relevant situations, many forces act simultaneously. Thus, there could be simultaneous fluxes of mass, charge, momentum and energy. Besides this, there could be significant interplay between the different forces and different fluxes. For example, mass flux is caused predominantly by a velocity gradient, as in the case of convection, or momentum and mass fluxes could also result from a temperature difference, as in the case of free convection. Let us look at examples of such situations in this chapter.

Now, let us first consider mass flux arising from multiple driving forces. The driving force for mass flux could be one or a combination of many i.e.

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a concentration gradient, an electrical voltage gradient, a pressure gradient, or a temperature gradient, indicated by subscripts c, E, p and T, respectively. When many forces act simultaneously, the total flux of the component i is the vectorial sum of the individual fluxes resulting from each driving force.

$$\vec{J}_i^{*} = \vec{J}_{i,c}^{*} + \vec{J}_{i,E}^{*} + \vec{J}_{i,p}^{*} + \vec{J}_{i,T}^{*} \tag{6-1}$$

Such situations often arise in biological systems. For example, when DNA or proteins are separated on gels, $\vec{J}_{i,c}^{*}$ and $\vec{J}_{i,E}^{*}$ would be relevant.

When multiple forces are simultaneously operational, the approach is to simultaneously solve the relevant conservation equations, which could be some or all of the following: equation of continuity (mass conservation), equation of motion (momentum conservation), the thermal energy equations (note that the thermal energy is not conserved), and the charge conservation equation (along with Maxwell's equations).

In many situations, the formulations and solutions can get highly complicated. An alternative approach is to use a less rigorous, but useful approach that involves transfer coefficients, i.e. conductances. For example

Mass flux = Mass transfer coefficient × (Δ Concentration)
Heat flux = Heat transfer coefficient × (Δ Temperature)

The above approach is useful for analysis, design and operation, and in some cases, provides good insights too. We will follow this approach for some complex situations that we will consider in this chapter.

6.1 Simultaneous Concentration Gradient and Electrical Potential Gradient

6.1.1 Mobility of Ions in Solution

When a system consisting of charged species or ions is placed in an electric field, the ions will experience a force due to the electric field and the force will result in an ion flux. The species velocity of the ions can be represented as the product of a force on a mole of ions (N mole^{-1}), f, and a quantity called the molar mechanical mobility (mole m (N s)$^{-1}$), u. Thus, the flux J_E^{*} due to the electric field is given, for one dimension, as

$$J_E^{*} = c\, v = c\, u\, f \tag{6.1.1-1}$$

Now

- In mechanical terms, Work done = Force × Distance
- In electrical terms, Work done = Charge × Potential difference

Equating the above two terms for the work done, we get

$$\begin{aligned}\text{Force per mole} &= \text{Charge per mole} \times (\text{Potential difference/Distance})\\ &= \text{Charge per mole} \times \text{Potential gradient}\end{aligned}$$

If the particles are charged with valence z, and the electric field intensity is $E = -\vec{\nabla}\mathbf{V}$ where $\mathbf{V}$ is the electric potential, the force on a mole of particles is given by

$$\begin{aligned}f &= -zF\vec{\nabla}\mathbf{V} = -zF\frac{d\mathbf{V}}{dx}(\text{in 1D}) \qquad (6.1.1\text{-}2)\\ &= zFE\end{aligned}$$

where F is Faraday's constant that establishes the equivalence between the chemical and electrical bases of looking at a flow of electrons. From a chemical point of view, a flow of electrons (particles) is considered as current, and hence the flow of the number of moles of electrons per unit time can be a unit of current. From an electrical point of view, the amount of charge per unit time is taken to be current. Thus, the equivalence can be worked out as

$$\begin{aligned}F = \left(\frac{\text{Electrons}}{\text{Mole}}\right)\times\left(\frac{\text{Charge}}{\text{Electron}}\right) &= (6.023\times10^{23})\times(1.6\times10^{-19})\\ &= 96487 \text{ coulomb mole}^{-1}\end{aligned}$$

From Eq. 6.1.1-1, in 1D

$$J_E^* = -cuzF\frac{d\mathbf{V}}{dx}$$

The above is true only for the electrical driving force. Normal diffusion would also be present because diffusion results from collision between molecules by virtue of thermal energy. Diffusion causes a flux of the charged species when there is an appropriate concentration gradient. Hence, from Eq. 6-1, the flux for the n^{th} ion can be written as

$$\begin{aligned}\vec{J}_n^* &= \vec{J}_{n,c}^* + \vec{J}_{n,E}^*\\ &= -D_n\frac{dc_n}{dx} - c_n u_n z_n F\frac{d\mathbf{V}}{dx} \qquad (6.1.1\text{-}3)\end{aligned}$$

The net charge flux (current density), I_n' i.e. charge per time per unit area, can be related to the net mass flux of the charged species, i.e. amount per time per unit area, J_n^* (see explanation of Faraday's constant above) as follows

$$I_n' = z_n F J_n^* \tag{6.1.1-4}$$

Substituting Eq. 6.1.1-3 into Eq. 6.1.1-4 gives

$$I_n' = - z_n F \left(D_n \frac{dc_n}{dx} + c_n u_n z_n F \frac{d\mathbf{V}}{dx} \right) \tag{6.1.1-5}$$

The above equation that gives the net ion flux when diffusion as well as mobility in an electric field are operational, is called the Nernst-Planck equation.

Einstein's relation gives an expression for ion diffusivity in terms of molar mechanical mobility as

$$D_n = u_n RT \tag{6.1.1-6}$$

Therefore

$$I_n' = - c_n u_n z_n F \left(\frac{RT}{c_n} \frac{dc_n}{dx} + z_n F \frac{d\mathbf{V}}{dx} \right)$$

or

$$I_n' = - c_n u_n z_n F \frac{d}{dx}(RT \ln c_n + z_n F\mathbf{V}) \tag{6.1.1-7}$$

At electro-diffusive equilibrium, the net fluxes of all ions are zero. Hence I_n' = 0; if only the x direction is considered, we can write

$$- c_n u_n z_n^2 F^2 \frac{d}{dx} \left(\frac{RT}{z_n F} \ln c_n + \mathbf{V} \right) = 0 \tag{6.1.1-8}$$

Now

$c_n \neq 0$ (a zero value implies absence of particles)
$u_n \neq 0$ (a zero value implies that the particles are fixed and cannot diffuse or move in an electric field)
$z_n \neq 0$ (a zero value implies uncharged particles)

Thus

$$\frac{d}{dx} \left(\frac{RT}{z_n F} \ln c_n + \mathbf{V} \right) = 0$$

The whole derivative being zero implies that the terms inside the bracket need to be a constant – a physically irrelevant situation with both c_n and $\mathbf{V}$ being constants. Therefore, let us see the situation as

$$\frac{d \ln c_n}{dx} = -z_n \beta \frac{d\mathbf{V}}{dx} \tag{6.1.1-9}$$

where

$$\beta = \frac{F}{RT}$$

Equation 6.1.1-9 can be integrated to give

$$c_n = c_{n,o} \exp\left[-z_n \beta (\mathbf{V} - \mathbf{V}_0)\right] \tag{6.1.1-10}$$

The subscript '*o*' indicates the point of reference for the potential.

Thus

$$(\mathbf{V} - \mathbf{V}_0) = -\frac{RT}{z_n F} \ln \frac{c_n}{c_{n,o}} \tag{6.1.1-11}$$

i.e. at electro-diffusive equilibrium, the spatial distribution of potential is proportional to the logarithm of the solute concentration. Equation 6.1.1-11 is very useful, and is referred to as the Nernst equation.

6.1.2 Mobility of Ions Across a Membrane

As mentioned in Chapter 5, our senses work because of the mobility of ions across neural cell membranes. Some proteins in the membrane act as 'passive' (not requiring energy) ion channels or 'active' (requiring energy) transporters for the transport of charged ions across the membranes; the charged species, due to their nature, cannot permeate through the non-polar lipid bilayer core at reasonable rates, although they can permeate at low rates.

When ions move across the biological membrane (charge flux across the membrane), at least two driving forces are at play, namely the potential difference and the concentration difference of the ion under consideration. The Nernst equation that we derived for ions in solution at electro-diffusive equilibrium must be valid here since the presence of the membrane is not expected to interfere with charge effects. If only one ion is being considered, say K^+, the Nernst equation applied to the membrane, i.e.

$$(\mathbf{V}_{\text{int}} - \mathbf{V}_{\text{ext}}) = -\frac{RT}{z_n F} \ln\left(\frac{c_{n,\text{int}}}{c_{n,\text{ext}}}\right) \tag{6.1.2-1}$$

(subscript 'int' denotes intracellular and 'ext' denotes extracellular) can be used to describe the equilibrium condition when there is no net transport of K^+, i.e. when the potential across the membrane is able to balance the driving force due to the concentration difference in K^+ between the inside and the outside of the cell. The K^+ ions that traverse the membrane are usually held on the other side of the membrane due to the charged head groups on both the extremities of the membrane cross-section that attract the ions to reside on the surface of the membrane. The difference in the charges on both sides of the membrane causes a potential difference to be set up across the membrane which is known as the *membrane potential*.

Example 6.1.2-1

A certain cell was found to have the following equilibrium concentrations of K^+ when the experiment was conducted at 37 °C: intracellular: 120 mM; extracellular 2.5 mM. Assuming that the membrane is permeable only to K^+, estimate the equilibrium membrane potential.

Solution

From Eq. 6.1.2-1

$$(\mathbf{V}_{\text{int}} - \mathbf{V}_{\text{ext}}) = -\frac{RT}{z_n F}\ln\left(\frac{c_{n,\text{int}}}{c_{n,\text{ext}}}\right)$$

where the LHS gives the membrane potential.

Substituting the values given and known, we get

$$(\mathbf{V}_{\text{int}} - \mathbf{V}_{\text{ext}}) = -\frac{8.314\times 310}{1\times 96487}\ln\left(\frac{120}{2.5}\right)$$

$$(\mathbf{V}_{\text{int}} - \mathbf{V}_{\text{ext}}) = -\,0.1034\ \text{V} = -\,103.4\ \text{mV}$$

Many ions move in and out of the cell through different channels, and contribute to the establishment of the membrane potential. It can be shown (see Plonsey and Barr, *Bioelectricity: A Quantitative Approach* on depletion) that a very small fraction of the charge in the solution (1.7×10^{-4}) is enough to set up a charge across the membrane. Also, the movement of charges across the membrane to set up the Nernst potential does not violate the electro neutrality principle in *solutions* (extracellular and intracellular solutions) for most cases since the number of charges involved is small, and they reside on the membrane side rather than in the solution. In some cases, however, the electro neutrality principle could be invalid, which may necessitate a more complex analysis.

The ions that are usually considered important are K^+ and Na^+ (and maybe Ca^{2+} in some cells such as the muscle cell). The initial developments in the first half of the 20th century considered only K^+ and Na^+ ions, and the results predicted by the models proposed then were close to the experimental values for the types of cells that were studied (Manchanda, personal communication). Thus, the earlier models did not consider the other ions that could pass passively across the cell membrane. For example, the chloride ion (Cl^-) can passively transit the cell membrane through its ion channel. However, usually the membrane potential is close to the Nernst potential of Cl^-. Thus, the Cl^- ion current is so small that it can be considered negligible. Also, note that the ions that cross the membrane through active transport, such as H^+, are not relevant for passive transport models. Nevertheless, active transport can be considered as an additional aspect to passive transport in appropriate models.

Hodgkin and Huxley were the first to assume that the fluxes of ions are independent of each other. Under this assumption, in equilibrium conditions, no net charge transport (by means of any ion) occurs across the membrane, and the ions are each under equilibrium. Application of Eq. 6.2-1 individually to each ion (say K^+, Na^+ and Ca^{2+}) across the membrane under equilibrium conditions, and the recognition that the membrane potential must be the same value even if different ion fluxes are considered (since all ions contribute to the establishment of the membrane potential), yields

$$\left(\frac{c_{\mathrm{K,int}}}{c_{\mathrm{K,ext}}}\right)^{\frac{1}{z_{\mathrm{K}}}} = \left(\frac{c_{\mathrm{Na,int}}}{c_{\mathrm{Na,ext}}}\right)^{\frac{1}{z_{\mathrm{Na}}}} = \left(\frac{c_{\mathrm{Ca,int}}}{c_{\mathrm{Ca,ext}}}\right)^{\frac{1}{z_{\mathrm{Ca}}}}$$

or

$$\left(\frac{c_{\mathrm{K,int}}}{c_{\mathrm{K,ext}}}\right) = \left(\frac{c_{\mathrm{Na,int}}}{c_{\mathrm{Na,ext}}}\right) = \left(\frac{c_{\mathrm{Ca,int}}}{c_{\mathrm{Ca,ext}}}\right)^{\frac{1}{2}} \qquad (6.1.2\text{-}2)$$

If chloride had been considered, the exponent for the ratio of intracellular to extracellular chloride concentrations would have been – 1.

The above equilibrium condition is referred to as the Donnan equilibrium. The membrane potential under Donnan equilibrium is called the *resting potential*.

Note that each ion would be at equilibrium across the membrane only at its Nernst potential. Nevertheless, in biological systems, the Donnan equilibrium is a very good approximation under most conditions. This is because the ion currents that arise due to non-equilibrium situations under resting potential conditions, and consequent charge loss/gain from/by the cell is reasonably small for the time scales normally associated with the cell dynamics that are studied.

6.1.3 Electrical Circuit Representation of a Membrane

The biological membrane, simplistically speaking, is made up of a bilayer of lipids and proteins. Some proteins act as ion channels for the transport of charged ions across the membranes; it may be recalled that charged species cannot permeate through the lipid bilayer at reasonable rates, although they do permeate at some small rates.

We also know that electrical phenomena result when charges are separated or charges can move independently. Any flow of charges is called a current (I) measured in amperes (Coulomb s^{-1}), and the direction depends on the charge sign: positive current in the direction of movement of positive charges.

Potential difference ($\Delta\mathbf{V}$) between the (+)ve and (–)ve poles, and the conductance (g) (or the inverse of resistance R) between them are related by the constitutive relationship, Ohm's law, as

$$\Delta\mathbf{V} = IR \text{ or } I = g(\Delta\mathbf{V}) \tag{6.1.3-1}$$

Each ion channel can be considered as a conductor (resistor) that spans the biological membrane. The total electrical conductance of the membrane is the sum of the conductance of the individual ion channels, acting in parallel.

Let us now focus on the other major part of the membrane, namely the lipid bilayer. As mentioned in Chapter 5, the nature of the bilayer and its surroundings makes it an electrical capacitor.

The capacitance C, i.e. the amount of charge Q that needs to be transferred from one conductor to another to result in a potential difference $\Delta\mathbf{V}$ is given by

$$C = \frac{Q}{\Delta\mathbf{V}} \tag{6.1.3-2}$$

For a parallel plate capacitor formed by two parallel plates, each of area A and separated by a distance d (this approximation is valid for a membrane that is stretched out to form a flat surface)

$$C = \frac{k\,\epsilon_o A}{d} \tag{6.1.3-3}$$

where k is dielectric constant and ϵ_o is permittivity of free space = 8.85 × 10^{-12} C $V^{-1}m^{-1}$.

The typical value for the capacitance of a cell membrane bilayer is about 1 μF cm^{-2}, which is large compared to the normal capacitances that are found in a typical electrical circuit.

Considering only the K^+ and Na^+ fluxes (independent of each other) across the membrane, it can be represented by an electrical circuit, as given

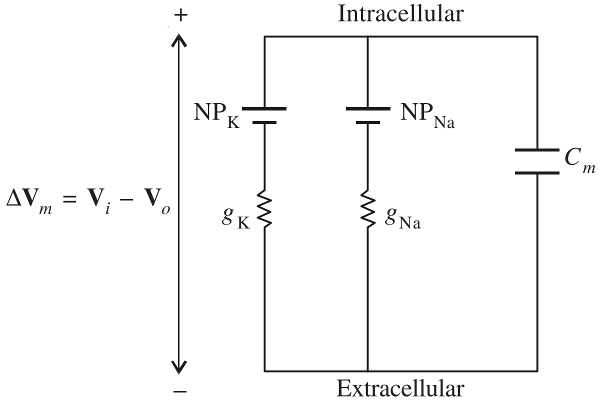


Fig. 6.1.3-1 Electrical circuit representation of a membrane

in Fig. 6.1.3-1. In the circuit, NP refers to the Nernst potential of the respective ions, C_m, the capacitance of the membrane, and $\Delta \mathbf{V}_m$, the membrane potential. The polarities of the batteries indicate the relative abundance of the ions at equilibrium for each ion across the membrane – K^+ concentration is higher in the intracellular space (say 120 mM) compared to that in the extracellular space (say 2 mM), and for Na^+, it is vice versa (say 5 mM and 110 mM in the intracellular and extracellular spaces, respectively).

The resting membrane potential is representative of a steady state, when there is no *net* ion flux (ion current) across the membrane. There could, however, be individual ion fluxes since the flux for a particular ion across the membrane would be zero only at *its* Nernst potential. Since the Nernst potential for each ion is different, there can be no common Nernst potential when the fluxes of all ions across the membrane cease. Nevertheless, at the resting membrane potential, there is no net ion flux across the membrane. Also, note that active transport of ions across the membrane through the transporter proteins, which occurs at much slower rates compared to that through the ion channels, is not included in the representation (or the model).

The ion currents (I_K or I_{Na}, for example) can be represented by the conductance, g, and the effective potential difference ($\Delta \mathbf{V}_m$ – NP).

$$I_K = g_K\ (\Delta \mathbf{V}_m - NP_K) \qquad (6.1.3\text{-}4)$$

$$I_{Na} = g_{Na}\ (\Delta \mathbf{V}_m - NP_{Na}) \qquad (6.1.3\text{-}5)$$

The above ion currents would be present irrespective of the electrical steady-state condition (resting potential) across the membrane.

Due to the capacitance, there would also be a capacitive current that can be represented by

$$I_C = C_m \frac{d(\Delta \mathbf{V}_m)}{dt} \tag{6.1.3-6}$$

At steady state (when the resting membrane potential is achieved), however, the capacitance current would be zero since the time derivative on the RHS of Eq. 6.1.3-6 would be zero. The sum of the other currents would also equal zero. Thus

$$g_{\mathrm{K}}\ (\Delta \mathbf{V}_{m,r} - \mathrm{NP_K}) + g_{\mathrm{Na}}\ (\Delta \mathbf{V}_{m,r} - \mathrm{NP_{Na}}) = 0$$

Therefore, the resting membrane potential can be calculated if the conductances and Nernst potentials of the ions involved are known, as follows

$$\Delta \mathbf{V}_{m,r} = \frac{g_{\mathrm{K}}\ \mathrm{NP_K} + g_{\mathrm{Na}}\ \mathrm{NP_{Na}}}{g_{\mathrm{K}} + g_{\mathrm{Na}}} \tag{6.1.3-7}$$

It can be expected that although ions are not permeable at significant rates across the lipid bilayer of the membrane, small, non-zero permeabilities of the ions do exist across the membrane due to the combined forces of the concentration gradient and a membrane potential (that is away from the Nernst potential of that ion). Thus, when the membrane is at rest, K^+ ions may move from the inside to the outside of the cell, and Na^+, vice versa. In addition, there is a protein called the Na^+-K^+ (sodium-potassium) pump on the membrane that transports 2 K^+ ions into the cell for every 3 Na^+ simultaneously pumped out. Energy (ATP) is needed to activate this pump, and hence it is an active transport; note that the active transport effects are not included in the models presented thus far. Therefore, the cell, when at rest, 'actively' maintains its distribution of K^+ and Na^+ ions across its membrane.

Example 6.1.3-1

In an animal neuron, the ion conductances at resting state were determined to be $g_{\mathrm{K}} = 0.42$ mS cm^{-2} and $g_{\mathrm{Na}} = 0.01$ mS cm^{-2}. The Nernst potentials for K and Na are respectively, – 74.7 mV and + 54.2 mV. Find the resting potential for the neuron.

Solution

From Eq. 6.1.3-7, we know that the resting membrane potential is given by

$$\Delta\mathbf{V}_{m,r} = \frac{g_\mathrm{K}\ \mathrm{NP_K} + g_\mathrm{Na}\ \mathrm{NP_{Na}}}{g_\mathrm{K} + g_\mathrm{Na}}$$

Substituting the values given, we get

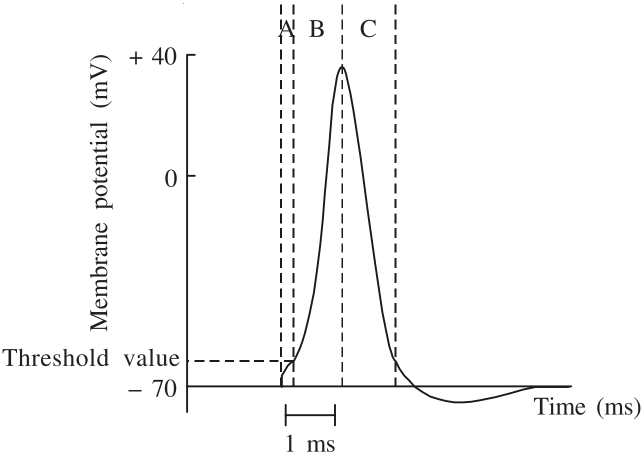
$$\Delta\mathbf{V}_{m,r} = \frac{0.42\times(-74.7)+0.01\times(+54.2)}{(0.42+0.01)} = -71.7\ \mathrm{mV}$$

6.1.4 Action Potential and Axial Current

Let us consider a cell (say a nerve cell) that is initially at the resting membrane potential. When this cell is stimulated, either through a signal received from another cell (say from eye neurons during the sight process through neurotransmitters at places called the synapses), or by artificial means through electrodes in an experimental set up, the sodium channels open up. As a result, $\mathrm{Na^+}$ ions move from the outside to the inside of the cell, causing the inside of the cell to become more positive. Thus, the membrane potential *moves away* from its resting value of say, – 70 mV (gets *depolarised*) and becomes more positive, as shown in Fig. 6.1.4-1. As more sodium ions come into the cell, more number of $\mathrm{Na^+}$ channels open up, and the membrane potential becomes more positive. When the membrane potential reaches about – 20 mV, the potassium channels open, and the $\mathrm{K^+}$ ions move from the inside to the outside of the cell. Nevertheless, the rate of $\mathrm{Na^+}$ entry is higher than the rate of $\mathrm{K^+}$ exit, and thus the membrane potential continues to become more positive until a value of + 40 mV is reached. At this value, the $\mathrm{Na^+}$ channels close, and the rate of $\mathrm{K^+}$ exit becomes higher. This leads to a decrease in the membrane potential and it *moves toward* its resting value (gets *repolarised*). When the membrane potential reaches suitable values, the $\mathrm{K^+}$ and $\mathrm{Na^+}$ channels close, and the membrane potential stabilises at its resting value of say, – 70 mV. This dynamic response of the membrane potential when the cell is 'stimulated' is called its *action potential.* A typical action potential is shown in Fig. 6.1.4-1.

The shape of the action potential curve is determined by many factors. For example, the dynamics of a $\mathrm{K^+}$ channel opening and an $\mathrm{Na^+}$ channel opening are different – the speed of the $\mathrm{Na^+}$ ion channel opening is faster. Moreover, $\mathrm{Na^+}$ channels have two gates, one on the extracellular side and the other on the intracellular side. While the outside gate opens when the

Fig. 6.1.4-1 The action potential and its relation to the opening and closing of membrane ion channels



During A: The Na^+ channels open, and Na^+ enters the cell.
During B: The Na^+ channels slowly close (inner gate closes slowly), and the K^+ channels open, enabling the K^+ ions to leave the cell. At the end of the B period, the Na^+ channels are completely closed.
During C: K^+ channels close toward the later part of C, and the Na^+ channels reset at the end of the C period.

depolarisation begins, the inside gate that is open even at the resting potential, starts closing slowly with increasing depolarisation. At a value of about + 40 mV, the inside gate of the Na^+ channel closes completely. While the Na^+ channel closes at + 40 mV due to the closure of its inside gate, the K^+ channel that has only one outside gate (on the extracellular side) opens up.

The time over which the action potential occurs is a few milliseconds. Further, the strength of the stimulus is important. If it is not high enough to cause the movement of the membrane potential beyond a critical value, say – 55 mV, then no action potential ensues. Beyond this magnitude of the stimulus, any value, however high (within some broad limits), causes the same magnitude of action potential. Thus, the action potential is a ‘all or none’ phenomenon, depending on whether the stimulus is above or below a certain value.

The Na^+ ions which move in at a certain location on the nerve cell can move intracellularly to other adjacent locations. Thus, they can activate the Na^+ channels in locations adjacent to the original location. Thus, action potentials arise in adjacent locations. This, in turn, leads to action potentials occurring in other adjacent locations along the length of the nerve cell. Thus, the action potential gets propagated along the length of the nerve cell – we can say that the original stimulus gets ‘transmitted’ along the nerve cell. This transmission can also be viewed as an *axial current* along the nerve cell and is known as the cable current.

6.1.5 Electrophoresis

Electrophoresis refers to the movement of charged particles/molecules in medium, under the effect of an electric field. As a technique, electrophoresis is widely used for the analysis of biological molecules such as DNA, RNA and proteins. The electric field is usually taken to be uniform and the charge is either naturally present on the molecules, or placed deliberately on them for certain types of analysis, say, for example to equalise the charges on all the molecules being analysed. The charged molecules of different sizes or charges move with different 'mobilities' through a viscous gel that is specially cast for the analysis – e.g. agarose gels are used for DNA analysis, and polyacrylamide gels for protein analysis.

As seen in Chapter 5, in the neutral state, the charges in the medium are surrounded by counter ions in the electrical double layer. When an electric field is applied, the counter ions in the double layer get disturbed; the charges respond to the applied electric field, and move toward the oppositely charged end.

In addition, when electrically neutral particles, such as whole cells, are subjected to a non-uniform electric field, the charge distribution in the particles is altered, and charge dipoles are induced. One part of the cell is charged differently from the other part, and hence an originally uncharged cell moves in the non-uniform electric field due to the induced polarisation. This process is called dielectrophoresis. The interested reader can refer to other specialised texts such as Pohl (1978) or Bakewell (2009) for more details on dielectrophoresis. In the remainder of this section, we will focus on electrophoresis, i.e. the movement of charged particles/molecules when the applied electric field is uniform.

In electrophoresis, both a concentration gradient and an electrical potential gradient exist, and therefore, as seen in Section 6.1.1, the flux is due to both diffusion and movement due to the electric field. However, the diffusivities of the biomolecules of interest such as nucleic acids or proteins, through a gel are negligibly small, compared to their electrical mobilities.

Therefore, let us consider only the movement due to the electric field in our analysis. Also, note that nucleic acids and proteins are typically placed as spots in the gel, and therefore, their movement can be treated as movement of particles through the gel. Only the salient results of the analysis will be directly presented in this section.

For simplicity, let us first consider only the charged particle (without the counter ions). Let the particle be spherical with a charge ze, and a radius r. The motion of the particle under an electric field in a gel will typically be slow enough for us to consider the motion to be in the Stokes' regime. When the particle moves at a terminal velocity, the forces due to the electric field on the particle $(ze)\ E$, and the frictional force for a particle moving in the Stokes' regime, $6\pi\mu rv$ (where μ is the medium (gel) viscosity) can be balanced to obtain

$$(ze)E = 6\pi\mu rv \tag{6.1.5-1}$$

The electrophoretic mobility m' which is the velocity per unit electric field strength v/E, can be written from Eq. 6.1.5-1 as

$$m' = \frac{(ze)}{6\pi\mu r} \tag{6.1.5-2}$$

Now, let us consider the counter ion cloud that surrounds the charged spherical particle. Let us assume that the cloud is a continuous (spherical) distribution of charges which has a different distribution when the uniform electric field is applied. Let the radius of the sphere in the presence of the uniform electric field be a. The electrostatic potential $\mathbf{V}$ at a distance d ($d > a$) in a medium of dielectric constant k (note that the dielectric constant is the ratio of the permittivity of the substance to the permittivity of free space, i.e. $\varepsilon/\varepsilon_0$) is given as

$$\mathbf{V} = \frac{ze}{kd} \tag{6.1.5-3}$$

Thus, there is a superposition of the fields and potentials from the modified spherical distribution of charges around the charged bioparticle, and the external source that is applied to cause movement. The solution of the approximate form of the Poisson-Boltzmann equation for this situation yields the modified potential $\mathbf{V}'$ as

$$\mathbf{V}' = \left(\frac{ze}{kd}\right)\left[\frac{\exp \kappa(a-d)}{1+\kappa a}\right] \tag{6.1.5-4}$$

where κ is the charge screening parameter that is also dependent on the ionic strength of the medium. An approximate mobility in this situation is given by

$$m'' = \frac{(ze)}{6\pi\mu r}\left[\frac{f(\kappa a)}{1+\kappa a}\right] \tag{6.1.5-5}$$

Different forms of the function $f(\kappa a)$ are available, e.g. the Henry function. Interested readers can refer to specialised journal articles such as Ohshima (2002).

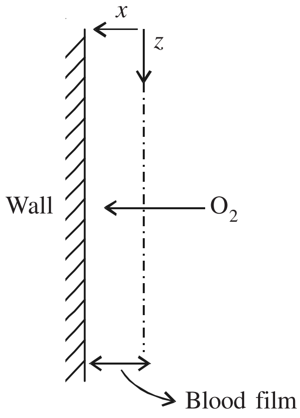


Fig. 6.2-1 Falling film blood oxygenation; convective transport of oxygen

6.2 Simultaneous Concentration Gradient and Velocity Gradient: Blood Oxygenators

Blood oxygenators are extensively used in hospitals when blood is taken out of a patient during surgical procedures and later returned to the patient. In the falling film type blood oxygenator, a blood film flows downward on a solid wall, while oxygen diffuses across the film and oxygenates the blood, as schematically represented in Fig. 6.2-1. Let us derive an expression for the rate of oxygen absorption into the blood film.

Usually, the rate of O_2 transport in the z (vertical) direction due to bulk flow is much higher than the diffusion in the same direction.

Thus

$$D_{\text{eff}} \frac{\partial^2 c_A}{\partial z^2} << v_z \frac{\partial c_A}{\partial z}$$

Nevertheless, there is no convective transport in the x direction and only diffusive transport occurs.

Thus, Eq. A2 from Table 2.3.2-1, the continuity equation, becomes

$$v_z \frac{\partial c_A}{\partial z} = D_{\text{eff}} \frac{\partial^2 c_A}{\partial x^2} \tag{6.2-1}$$

We have also neglected the reaction term above, i.e. the reaction between oxygen and haemoglobin has been assumed to be negligible.

The boundary conditions are

At $x = 0$, $c_A = c_{Ai}$ (oxygen concentration at the gas-liquid interface) (6.2-2)

At $x = \delta$, $\dfrac{\partial c_A}{\partial x} = 0$ (at the wall, i.e. $x = \delta$, oxygen cannot penetrate the wall) (6.2-3)

At $z = 0$, $c_A = c_{Ao}$ (oxygen concentration in the deoxygenated blood entering at the top of the plate) (6.2-4)

Let us consider a thin uniform film. When we compare this with the flow over the inclined surface (Bostwick viscometer) that we considered in Chapter 3, we can assume

$$v_z \neq f(z) = v_o$$

Let us define some non-dimensional variables as

$$\Theta(\eta, \varphi) = \frac{c_{Ai} - c_A(x,z)}{c_{Ai} - c_{Ao}} \tag{6.2-5}$$

$$\eta = \frac{x}{\delta} \tag{6.2-6}$$

$$\varphi = \frac{Z\,D_{\text{eff}}}{v_o\,\delta^2} \tag{6.2-7}$$

In terms of the non-dimensional variables, the differential equation and the boundary conditions become

$$\frac{\partial \Theta}{\partial \varphi} = \frac{\partial^2 \Theta}{\partial \eta^2} \tag{6.2-8}$$

Boundary conditions are

$$\text{At } \eta = 0,\ \Theta = 0 \tag{6.2-9}$$

$$\text{At } \eta = 1, \frac{\partial \Theta}{\partial \xi} = 0 \tag{6.2-10}$$

$$\text{At } \varphi = 0,\ \Theta = 1 \tag{6.2-11}$$

Invoking the separation of variables method, let us write

$$\Theta\ (\eta, \varphi) = X(\eta)\ Y(\varphi) \tag{6.2-12}$$

Using a procedure similar to that employed in Chapter 3 for solving unsteady state flow situations in a pipe, we get

$$Y = A \exp\ (-\ b^2\varphi) \tag{6.2-13}$$

and

$$X = B_1 \sin b\ \eta + B_2 \cos b\ \eta \tag{6.2-14}$$

Using the boundary condition 1, Eq. 6.2-9, cosine term = 0; using the boundary condition 2, Eq. 6.2-10

$$b = \left(n - \frac{1}{2} \right) \pi$$

where $n = 0, \pm 1, \pm 2, \ldots,$ for B_1 to be non-zero. Otherwise, a trivial equation, 0 = 0, would result.

Orthogonality: Two functions $f_m(x)$ and $f_n(x)$ are said to be orthogonal over an interval (a, b) if

$$\int_a^b f_m(x)\, f_n(x) dx = 0$$

For example

$$\int_0^1 \sin m\Pi x \sin n\Pi x\, dx = 0 \quad \text{when } m \neq n \text{ or } m = n = 0$$

$$\text{when } m = n, \text{ but} \neq 0$$

Using the orthogonality relationship, we get

$$\Theta(\eta, \varphi) = \frac{4}{\Pi} \sum_{n=1}^{\infty} \frac{1}{2n-1} \sin \left(n - \frac{1}{2} \right) \pi\eta \exp \left\{ -\left(n - \frac{1}{2} \right)^2 \pi^2 \varphi \right\} \qquad (6.2\text{-}15)$$

If L is the length of the film along the wall (longitudinal) and B is wall width, the rate of oxygen absorbed W_A in terms of the regular dimensional variables is

$$W_A = \int_0^B \int_0^L J^*_{Ax} \Big|_{x=0} dz\, dy \qquad (6.2\text{-}16)$$

where

$$J^*_{Ax} = \text{Diffusive flux} = -\, D_{\text{eff}} \frac{\partial c_A}{\partial x}$$

Thus

$$W_A = \frac{8BLv_z(c_{Ai} - c_{Ao})}{\Pi^2} \sum_{n=1}^{\infty} \frac{1}{(2n-1)^2} \left\{ 1 - \exp \left\{ -\left(n - \frac{1}{2} \right)^2 \frac{\Pi^2 L D_{\text{eff}}}{v_o \delta^2} \right\} \right\}$$

(6.2-17)

The average oxygen concentration $c_{A,av}$

$$c_{A,av} = c_{Ai} - (c_{Ai} - c_{Ao}) \frac{8}{\Pi^2} \sum_{n=1}^{\infty} \frac{1}{(2n-1)^2} \exp \left\{ -\left(n - \frac{1}{2} \right)^2 \frac{\Pi^2 L D_{\text{eff}}}{v_o \delta^2} \right\}$$

(6.2-18)

The above model, however, falls short in agreement with experimental data. This is because the reaction between oxygen and haemoglobin has not been considered. Also, blood has been approximated as a Newtonian fluid.

6.2.1 The Transfer Coefficient Approach: Inter-phase Oxygen Supply to Bioreactors

When mass or heat flux (or mass and heat flux) occur simultaneously with momentum flux, the relevant balances (mass or/and energy and momentum) are valid and need to be solved together. In many situations e.g. in a stirred bioreactor, the flow fields are not clearly defined and this adds to the complexity.

Thus, an alternative approach would be useful, especially for design and operation. The transfer coefficient approach is one such method which helps in designing and operating macro-systems, and allows for a certain level of analysis/understanding.

In general, the following representation is used in the approach.

$$\text{Flux} = \text{Transfer coefficient} \times \text{Driving force} \tag{6.2.1-1}$$

i.e.

$$\text{Mass flux} = \text{Mass transfer coefficient} \times \text{Concentration difference} \tag{6.2.1-2}$$

$$\text{Heat flux} = \text{Heat transfer coefficient} \times \text{Temperature difference} \tag{6.2.1-3}$$

Different transfer coefficients (say, mass transfer coefficient) can be used depending on the situation. For example

In a liquid phase

$$N_A = k_c(c_{A1} - c_{A2}) \tag{6.2.1-4}$$

$$= k_x(x_{A1} - x_{A2}) \tag{6.2.1-5}$$

In a gas phase

$$N_A = k_g(p_{A1} - p_{A2}) \tag{6.2.1-6}$$

$$= k_y(y_{A1} - y_{A2}) \tag{6.2.1-7}$$

We will look at heat transfer coefficient in a later section.

The mass transfer coefficients are especially useful when we quantify mass transfer across phases. Recall from thermodynamics that for mass

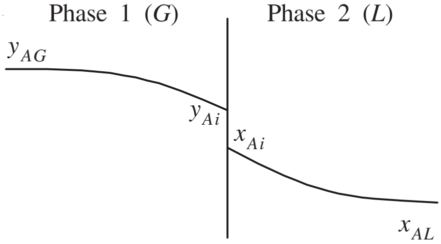


Fig. 6.2.1-1 The concentration profiles in the gas and liquid phases during gas-liquid interphase transport of a species (say oxygen)

transfer, it is the difference in chemical potentials that provides the actual driving force. In single phase, we can approximate chemical potential difference to concentration difference. But across phases (interphase), this approximation becomes difficult. More importantly, chemical potentials are not easy to measure, and use of a suitable concentration for chemical potential becomes easier with the use of a mass transfer coefficient. There are many methods, including experiments, correlations and theories, to find the transfer coefficients.

Let us consider the transfer of a species *A* across two phases, 1 and 2, represented as 1/2. There are several possibilities. $G|L$ represents the transfer of *A* between a gas phase and a liquid phase; $S|L$ represents the transfer of *A* between a solid phase and a liquid phase; $L|L$ represents the transfer of *A* between two liquid phases that are immiscible, and so on.

Let us consider $G|L$ for elaboration here (Fig. 6.2.1-1). The basal representations remain the same whatever be the two phases under consideration.

The flux of mass transfer of *A* in the gas phase

$$= k_y(y_{AG} - y_{Ai}) \tag{6.2.1-8}$$

where k_y is the gas phase mass transfer coefficient.

The flux in the liquid phase

$$= k_x(x_{Ai} - x_{AL}) \tag{6.2.1-9}$$

Lewis and Whitman (1924) proposed that resistances to mass transfer reside only in the phases – across the interface *i* there is no resistance for mass transfer. Consequently, the concentrations, y_{Ai} and x_{Ai} are equilibrium concentrations. This has been experimentally verified.

As interphase concentrations are not easy to measure, we use bulk concentrations and an 'overall mass transfer coefficient'.

However, *x* and *y* are concentrations in different phases (they are different quantities and the denominator volumes are also different), and hence algebraic operations cannot be done with them. The way around this difficulty is to use the concentration in one phase that is supposed to be in equilibrium with the bulk concentration in the other phase.

For example, in one $G|L$ transport case

$$N_A = K_y (y_{AG} - y_A^*) \tag{6.2.1-10}$$

where y_A^* is the concentration in the gas phase that will be in equilibrium when the liquid phase concentration is x_{AL}; the corresponding gas phase concentration is y_A^*.

K_y = Overall mass transfer coefficient for transfer from G to L phases

N_A can also be represented as

$$N_A = K_x (x_A^* - x_{AL}) \tag{6.2.1-11}$$

where x_A^* is the liquid phase concentration in equilibrium with y_{AG}.

At steady state, there should be no accumulation at the interface. Therefore, the flux of A reaching the interface = flux of A leaving the interface.

$$k_y(y_{AG} - y_{Ai}) = k_x(x_{Ai} - x_{AL}) = N_A \tag{6.2.1-12}$$

Also, the flux, N_A, can be written in terms of the overall mass transfer coefficients. The two expressions need to be the same because they represent the same flux.

$$N_A = K_y (y_{AG} - y_A^*) = K_x (x_A^* - x_{AL}) \tag{6.2.1-13}$$

If the equilibrium curve is linear, or can be considered to be piece-wise linear in the region of interest

$$y_{Ai} = m\ x_{Ai} \tag{6.2.1-14}$$

$$y_A^* = m\, x_{AL} \tag{6.2.1-15}$$

From Eq. 6.2.1-12

$$y_{AG} - y_{Ai} = \frac{N_A}{k_y} \tag{6.2.1-16}$$

$$x_{Ai} - x_{AL} = \frac{N_A}{k_x} \tag{6.2.1-17}$$

We can write Eq. 6.2.1-17 as

$$\frac{y_{Ai} - y_A^*}{m} = \frac{N_A}{k_x}$$

or

$$y_{Ai} - y_A^* = N_A \frac{m}{k_x} \tag{6.2.1-18}$$

Adding Eqs. 6.2.1-16 and 6.2.1-18, we get

$$y_{AG} - y_A^* = N_A\left[\frac{1}{k_y} + \frac{m}{k_x}\right] \qquad (6.2.1\text{-}19)$$

Also, from Eq. 6.2.1-13, we get

$$y_{AG} - y_A^* = \frac{N_A}{K_y} \qquad (6.2.1\text{-}20)$$

Thus

$$\frac{1}{K_y} = \frac{1}{k_y} + \frac{m}{k_x} \qquad (6.2.1\text{-}21)$$

Alternatively, if we consider the other overall coefficient, we can write

$$y_{AG} - y_{Ai} = \frac{N_A}{k_y} \qquad (6.2.1\text{-}22)$$

Therefore

$$m(x_A^* - x_{Ai}) = \frac{N_A}{k_y}$$

or

$$x_A^* - x_{Ai} = \frac{N_A}{mk_y} \qquad (6.2.1\text{-}23)$$

Also from Eq. 6.2.1-12, we get

$$x_{Ai} - x_{AL} = \frac{N_A}{k_x} \qquad (6.2.1\text{-}24)$$

Adding Eqs. 6.2.1-22 and 6.2.1-23, we get

$$x_A^* - x_{AL} = N_A\left[\frac{1}{mk_y} + \frac{1}{k_x}\right] \qquad (6.2.1\text{-}25)$$

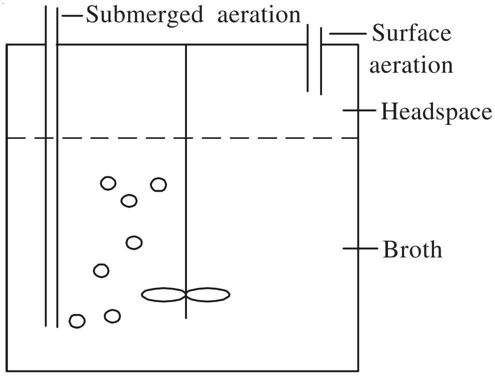
Also, from Eq. 6.2.1-13

$$x_A^* - x_{AL} = \frac{N_A}{K_x} \qquad (6.2.1\text{-}26)$$

From Eqs. 6.2.1-26 and 6.2.1-25, we get

$$\frac{1}{K_x} = \frac{1}{mk_y} + \frac{1}{k_x} \qquad (6.2.1\text{-}27)$$

Fig. 6.2.1-2 A schematic of a stirred bioreactor



If m is large

$$\frac{1}{K_x} \approx \frac{1}{k_x}$$

i.e. the overall resistance = resistance in the liquid phase. This implies that the mass transfer flux is determined by the gas side mass transfer flux.

Now, using the overall mass transfer coefficient (Eq. 6.2.1-13)

$$\text{Flux} = \frac{\text{Moles transferred}}{\text{Area} - \text{Time}} = K_x(x_A^* - x_{AL})$$

Thus

$$\begin{aligned}\text{The mass transfer rate} &= \frac{\text{Moles transferred}}{\text{Time}} \\ &= K_x A(x_A^* - x_{AL})\end{aligned}$$

where A is interfacial area.

Also

$$\begin{aligned}\frac{\text{Moles transferred}}{\text{Volume} - \text{Time}} &= K_x \frac{A}{V}(x_A^* - x_{AL}) \\ &= K_x a(x_A^* - x_{AL}) \qquad (6.2.1\text{-}28)\end{aligned}$$

where a is interfacial area per unit volume.

Since the interfacial area cannot be easily measured, $K_x a$ is measured as a single variable. In bioreactors, the volumetric oxygen transfer coefficient ($K_x a$ for oxygen) is referred to as '$K_l a$'. $K_l a$ is an important parameter that is determined before bioreactor operation. It provides a measure of the bioreactor's volumetric oxygen transfer capacity.

Bioreactors use either surface aeration or submerged aeration to supply oxygen to the culture in them (Fig. 6.2.1-2).

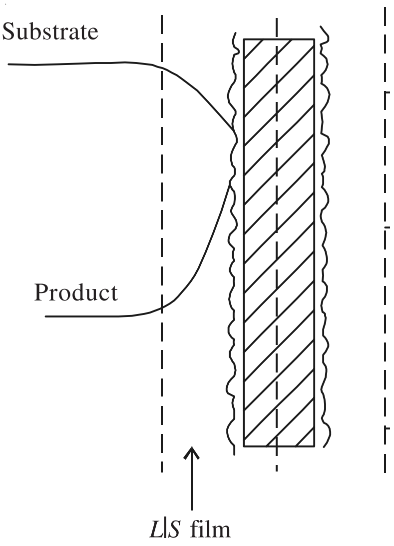


Fig. 6.2.2-1 Reaction occurring with the enzyme immobilised on the surface of a slab. The substrate transfers from the liquid to the slab surface, through the *L*|*S* film. The product formed on the surface due to the enzymatic reaction gets transferred to the bulk liquid

In surface aeration, the oxygen is transferred from the air in the headspace to the liquid across the gas-liquid interface that separates the broth from the headspace. In submerged aeration, the oxygen is transferred across the bubble surface to the liquid. The rate of oxygen transfer possible with submerged aeration is usually much larger than that possible with headspace aeration. As seen in Chapter 1, the liquid phase oxygen supply strategy (LPOS) can be used to improve the oxygen availability to bioreactors.

6.2.2 The Transfer Coefficient Approach: Immobilised Enzyme Reaction Kinetics

In Chapter 2, we considered the case when diffusion played a major role in determining the rate of a reaction that occurs inside a porous pellet. Let us now consider a reaction on the surface of a non-porous surface in a fluid when there is mass transport of reactants from the bulk fluid.

Take an enzyme immobilised on a slab that is non-porous (Fig. 6.2.2-1). The intrinsic enzyme kinetics is Michaelis-Menten and the reaction occurs on the surface of the slab. Let us derive an expression for the process rate at steady state.

Since it is a slab, let us consider rectangular coordinates. Since the flow condition could be undefined, let us take a transfer coefficient approach to represent the flux. It can be written as

$$N_S = k'_s\,(S_o - S) \tag{6.2.2-1}$$

where N_S is flux, k'_s is mass transfer coefficient, S_o is bulk substrate concentration and S is $S|L$ interface substrate concentration. k'_s can be obtained through correlations that are found in literature.

At steady state, substrate cannot accumulate at the catalyst bulk interface. The rate at which the substrate reaches the interface must equal the rate at which it gets consumed. That is

$$k_s(S_o - S) = \frac{v'_{\max} S}{K'_m + S} = v_{\text{app}} \tag{6.2.2-2}$$

where k_s is mass transfer coefficient on a volumetric basis, K'_m and $v'_{\max}$ are Michaelis-Menten constants and v_{app} is apparent velocity of the process.

Let us define some non-dimensional variables as

$$x = \frac{S}{S_o} \tag{6.2.2-3}$$

$$\text{Da} = \text{Damköhler number} = \frac{v'_{\max}}{k_s S_o} = \frac{\text{Mass reaction rate}}{\text{Maximum mass transfer rate}} \tag{6.2.2-4}$$

If

- Da << 1, the reaction is slow, and the process is reaction limited.
- Da >> 1, the mass transfer is slow, and the process is mass transfer limited.

$$K' = \frac{K'_m}{S_o} \tag{6.2.2-5}$$

Substituting the above variables in Eq. 6.2.2-2, we get

$$\frac{1-x}{\text{Da}} = \frac{x}{K' + x} = \frac{v_{\text{app}}}{v'_{\max}} \tag{6.2.2-6}$$

Solving $\dfrac{1-x}{\text{Da}} = \dfrac{x}{K' + x}$, we get

$$x = \frac{\beta}{2}\left(-1 \pm \sqrt{1 + \frac{4K'}{\beta^2}}\right) \tag{6.2.2-7}$$

where $\beta = \text{Da} + K' - 1$.

Inside the bracket in Eq. 6.2.2-7, we use + for $\beta > 0$ and – for $\beta < 0$. v_{app} is process rate and can be obtained by substituting x in Eq. 6.2.2-6.

An ‘effectiveness factor’ can be defined as

$$\xi_g = \frac{\text{Observed reaction rate}}{\text{Reaction rate in the absence of mass transfer resistance (i.e. } S = S_o)} \tag{6.2.2-8}$$

The effectiveness factor can be used to evaluate the effect of mass transfer on process rates. By substituting $S = S_o$ in Eq. 6.2.2-6 for the denominator, we get

$$\xi_g = \frac{\dfrac{x}{K' + x}}{\dfrac{1}{K' + 1}} \tag{6.2.2-9}$$

When Da → 0, $x \to 1$ i.e. when the process is totally reaction limited, $\xi_g \to 1$. This implies that

$$v_{\text{app}} = \frac{v'_{\max} S_o}{K'_m + S_o}$$

i.e. the process kinetics is the same as intrinsic kinetics. Mass transfer rate does not affect the process rate.

On the other hand, when Da → ∞, i.e. when the process is totally mass transfer limited, by substituting Eq. 6.2.2-7 in the RHS of Eq. 6.2.2-6 (and noting that K' needs to be finite), we get

$$\xi_g \to \frac{1 + K'}{\text{Da}}$$

and

$$v_{\text{app}} = k_s S_o$$

i.e. there is no trace of reaction kinetics in the process kinetics. It is totally mass transfer limited.

6.3 Simultaneous Temperature Gradient and Velocity Gradient: Heat Transfer to Fluid Flowing in a Long Circular Tube Under Laminar Flow Conditions

A protein solution needs to be heated as part of a certain analysis in a small scale. The micro-device utilised for the analysis uses a comparatively long, horizontal, metal tube with a small diameter. The electrically heated tube wall heats the solution that passes through it in laminar flow. The heat flux at the tube wall can be assumed to be constant. Find the temperature as a function of distance along the tube.

Note that

$$v_r = 0,\ v_\theta = 0,\ Q_\theta = 0$$

Also let us assume constancy of physical properties and neglect viscous dissipation (negligible compared to heating effects).

The relevant equations are (from the appropriate tables in the earlier chapters)

Equation of continuity

$$\frac{\partial v_z}{\partial z} = 0 \tag{6.3-1}$$

Equation of motion

$$\rho v_z \frac{\partial v_z}{\partial z} = -\frac{\partial p}{\partial z} + \mu\left[\frac{1}{r}\frac{\partial}{\partial r}\left(r\frac{\partial v_z}{\partial r}\right) + \frac{\partial^2 v_z}{\partial z^2}\right] \tag{6.3-2}$$

Equation of energy

$$\rho C_V v_z \frac{\partial T}{\partial z} = k\left[\frac{1}{r}\frac{\partial}{\partial r}\left(r\frac{\partial T}{\partial r}\right) + \frac{\partial^2 T}{\partial z^2}\right] + \mu\left(\frac{\partial v_z}{\partial r}\right)^2 \tag{6.3-3}$$

Using Eq. 6.3-1 i.e. $\frac{\partial v_z}{\partial z} = 0$, therefore $\frac{\partial}{\partial z}\left(\frac{\partial v_z}{\partial z}\right) = 0$ and Eq. 6.3-2 becomes

$$\frac{\partial p}{\partial z} = \mu\left[\frac{1}{r}\frac{\partial}{\partial r}\left(r\frac{\partial v_z}{\partial r}\right)\right] \tag{6.3-4}$$

We have seen in Chapter 3 that the solution of the above equation is

$$v_z = \frac{(p_o - p_L)R^2}{4\mu L}\left[1 - \left(\frac{r}{R}\right)^2\right] \tag{6.3-5}$$

Note that in Chapter 3 we had considered laminar flow down a vertical tube, and hence we needed to consider $P = p - \rho gh$. The reader is encouraged to derive the equation for a horizontal tube, and thus be convinced that $P = p$ for the case of laminar flow in a horizontal tube.

Substituting Eq. 6.3-5 into the energy Eq. 6.3-3, and differentiating Eq. 6.3-5, we get

$$\rho C_V \frac{(p_o - p_L)R^2}{4\mu L}\left[1-\left(\frac{r}{R}\right)^2\right]\frac{\partial T}{\partial z} = k\left[\frac{1}{r}\frac{\partial}{\partial r}\left(r\frac{\partial T}{\partial r}\right)+\frac{\partial^2 T}{\partial z^2}\right]+\mu\left(\frac{\partial v_z}{\partial r}\right)^2 \tag{6.3-6}$$

Usually, heat conduction in the z direction $\left(\text{term containing } \frac{\partial^2 T}{\partial z^2}\right)$ is negligible compared to the convective term $\left(\text{terms containing } \frac{\partial T}{\partial z}\right)$. Therefore, after differentiating Eq. 6.3-5 to get the last term in terms of the relevant variables, we can write

$$\rho C_V v_{z,\max}\left[1-\left(\frac{r}{R}\right)^2\right]\frac{\partial T}{\partial z} = k\frac{1}{r}\frac{\partial}{\partial r}\left(r\frac{\partial T}{\partial r}\right)+\left(\frac{(p_o - p_L)R^2}{4\mu L}\right)^2\frac{1}{R^4}4r^2$$

or

$$\rho C_V v_{z,\max}\left[1-\left(\frac{r}{R}\right)^2\right]\frac{\partial T}{\partial z} = k\frac{1}{r}\frac{\partial}{\partial r}\left(r\frac{\partial T}{\partial r}\right)+\frac{4v_{z,\max}^2}{R^4}r^2$$

Now, viscous dissipation (the phenomenon that contributes to the last term on the RHS of Eq. 6.3-6) is important only when the velocity gradients are large. If the velocity gradients are not large, the term, $\mu\left(\frac{\partial v_z}{\partial r}\right)^2$ can be dropped, and the relevant equation becomes

$$\rho C_V v_{z,\max}\left[1-\left(\frac{r}{R}\right)^2\right]\frac{\partial T}{\partial z} = k\frac{1}{r}\frac{\partial}{\partial r}\left(r\frac{\partial T}{\partial r}\right) \tag{6.3-7}$$

Now, the boundary conditions are

$$\text{At } r = 0,\ T = \text{finite} \tag{6.3-8}$$

$$\text{At } r = R,\ -k\frac{\partial T}{\partial r} = Q_1 \tag{6.3-9}$$

$$\text{At } z = 0,\ T = T_o \text{ (for all } r) \tag{6.3-10}$$

Let us introduce some non-dimensional groups

$$\theta = \frac{T - T_o}{Q_1 \dfrac{R}{k}} \tag{6.3-11}$$

$$\xi = \frac{r}{R} \tag{6.3-12}$$

$$\zeta = \frac{z\,k}{\rho C_V v_{z,\max} R^2} \tag{6.3-13}$$

Note that

$$\zeta = \left(\frac{z}{R}\right)\left(\frac{\mu}{D\,v_{z,\text{avg}}\,\rho}\right)\left(\frac{k}{\mu C_V}\right) = \left(\frac{z}{R}\right)\left(\frac{1}{N_{\text{Re}}}\right)\left(\frac{1}{N_{\text{Pr}}}\right)$$

by expressing the Reynolds number in terms of the diameter and the average velocity (the factor of 2 gets cancelled). The Reynolds number and the Prandtl number appear in most forced convection situations.

Thus, Eq. 6.3-7 becomes

$$(1-\xi^2)\frac{\partial \theta}{\partial \zeta} = \frac{1}{\xi}\frac{\partial}{\partial \xi}\left(\xi \frac{\partial \theta}{\partial \xi}\right) \tag{6.3-14}$$

Boundary conditions are

$$\text{At } \xi = 0,\ \theta = \text{finite} \tag{6.3-15}$$

$$\text{At } \xi = 1,\ -\frac{\partial \theta}{\partial \xi} = 1 \tag{6.3-16}$$

$$\text{At } \zeta = 0,\ \theta = 0 \tag{6.3-17}$$

In the limiting case (for large ζ), an analytical solution exists

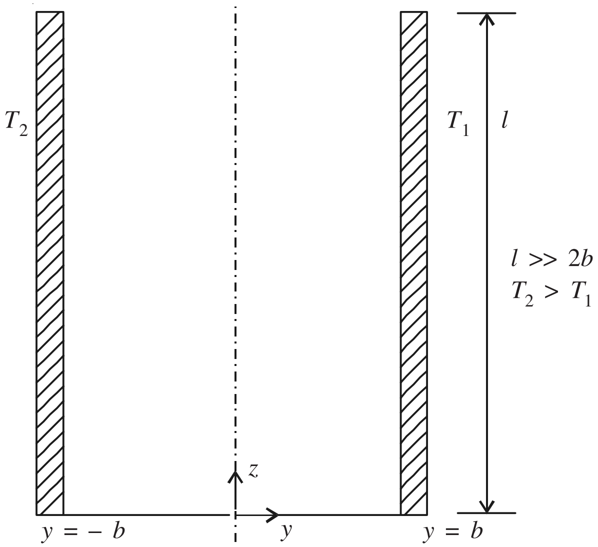
$$\theta = -4\zeta - \xi^2 + \frac{1}{4}\xi^4 + \frac{7}{24} \tag{6.3-18}$$

6.3.1 Momentum Flux Induced by Thermal Force: Free Convection

A possible strategy to achieve the desired heating of temperature sensitive food/solutions, under certain conditions, is to pass it and hold it for a certain period of time in a thin box of rectangular cross section. The box is vertically placed (Fig. 6.3.1-1). One of the two larger surfaces of the box is held at T_2 and the surface opposite to it is held at T_1. The length of the largest side is much greater than the distance ($2b$) between the surfaces. Let us find the distributions of temperature and velocity in the food solution at steady state.

Due to the temperature gradient, and the consequent density differences, the fluid near the hotter wall will rise and the fluid near the colder wall will descend. Let us assume that the volumetric flow rate in the upward moving stream is the same as that in the downward moving stream.

Fig. 6.3.1-1 The set up to heat temperature sensitive substances with two surfaces at different temperatures and a fluid in between them



Since it is given that the plates are held at constant temperatures, the temperature does not vary in the z direction, and we can assume $T = f(y)$ alone. Let us also assume that the fluid is Newtonian.

It is preferable to use rectangular coordinates in this case.

From Table 4-1, Eq. A, we get

$$0 = k\frac{d^2T}{dy^2} \tag{6.3.1-1}$$

Boundary conditions are

$$\text{At } y = -b,\ T = T_2 \tag{6.3.1-2}$$

$$\text{At } y = b,\ T = T_1 \tag{6.3.1-3}$$

Solving by integrating twice

$$\frac{dT}{dy} = c_1$$

$$T = c_1 y + c_2$$

Using the boundary conditions, we can get

$$T_2 = c_1(-b) + c_2$$

$$T_1 = c_1(b) + c_2$$

$$c_2 = \frac{T_2 + T_1}{2} = \text{say, } T_m$$

$$c_1 = \frac{T_1 - T_m}{b} = \frac{2T_1 - T_1 - T_2}{2b} = \frac{T_1 - T_2}{2b}$$

Therefore

$$T = \frac{T_1 - T_2}{2b} y + T_m$$

$$T = T_m - \frac{\Delta T}{2}\left(\frac{y}{b}\right) \tag{6.3.1-4}$$

where $\Delta T = T_2 - T_1$. Equation 6.3.1-4 gives the temperature profile.

To find the velocity profile, let us use Eq. C2 of Table 3.4-1. The equation reduces to

$$\mu \frac{d^2 v_z}{dy^2} = \frac{dp}{dz} + \rho g \tag{6.3.1-5}$$

Here, we cannot ignore the dependence of ρ on T because it is the difference in ρ that is causing the flow. To address the same, let us expand ρ in a Taylor's series in T about some reference temperature T_{ref}.

$$\rho = \rho\,|_{T\,\mathrm{ref}} + \left(\frac{\partial \rho}{\partial T}\right)\Bigg|_{T_{\mathrm{ref}}} (T - T_{\mathrm{ref}}) + \text{ Higher order terms (HOT)}$$

$$= \rho_{\mathrm{ref}} + \rho_{\mathrm{ref}} \beta_{\mathrm{ref}} (T - T_{\mathrm{ref}}) + \mathrm{HOT} \tag{6.3.1-6}$$

where

$$\beta = \frac{1}{\hat{V}}\left(\frac{\partial \hat{V}}{\partial T}\right)_p = \frac{1}{\left(\frac{1}{\rho}\right)}\left(\frac{\partial\left(\frac{1}{\rho}\right)}{\partial T}\right)_p = -\frac{1}{\rho}\left(\frac{\partial \rho}{\partial T}\right)_p \tag{6.3.1-7}$$

β_{ref} is evaluated at T_{ref}.

If we assume that HOT contribute negligibly, and substitute the first two terms of Eq. 6.3.1-6 in Eq. 6.3.1-5, we get

$$\mu \frac{d^2 v_z}{dy^2} = \frac{dp}{dz} + \rho_{\mathrm{ref}}\, g - \rho_{\mathrm{ref}} \beta_{\mathrm{ref}}\, g (T - T_{\mathrm{ref}}) \tag{6.3.1-8}$$

The pressure gradient is solely due to the weight of the fluid in the slot (let us assume that the temperature dependence of the pressure gradient can be ignored for a first estimate). Therefore

$$\frac{dp}{dz} = -\rho_{\mathrm{ref}}\, g$$

Thus

$$\mu \frac{d^2 v_z}{dy^2} = -\rho_{\text{ref}}\beta_{\text{ref}}\, g(T - T_{\text{ref}}) \tag{6.3.1-9}$$

By substituting the temperature distribution (Eq. 6.3.1-4) into Eq. 6.3.1-9 we get

$$\mu \frac{d^2 v_z}{dy^2} = -\rho_{\text{ref}}\beta_{\text{ref}}\, g\left((T_m - T_{\text{ref}}) - \frac{\Delta T}{2}\left(\frac{y}{b}\right)\right) \tag{6.3.1-10}$$

The boundary conditions are

$$\text{At } y = -b,\ v_z = 0$$

$$\text{At } y = b,\ v_z = 0$$

The solution is

$$v_z = \frac{\rho_{\text{ref}}\beta_{\text{ref}}\, g\, b^2 \Delta T}{12\mu}[\eta^3 - A\eta^2 - \eta + A] \tag{6.3.1-11}$$

where $A = \dfrac{6(T_m - T_{\text{ref}})}{\Delta T}$ and $\eta = \dfrac{y}{b}$.

We know that the net flow in the z direction = 0. Or in other words

$$\int_{-1}^{1} v_z\, d\eta = 0 \tag{6.3.1-12}$$

Substituting Eq. 6.3.1-11 in Eq. 6.3.1-12, we get

$$-\frac{2}{3}A + 2A = 0$$

$\Rightarrow A = 0$, or in other words

$$T_m = T_{\text{ref}} \tag{6.3.1-13}$$

Thus, the velocity distribution

$$v_z = \frac{\rho_{\text{ref}}\beta_{\text{ref}}\, g\, b^2 \Delta T}{12\mu}(\eta^3 - \eta) \tag{6.3.1-14}$$

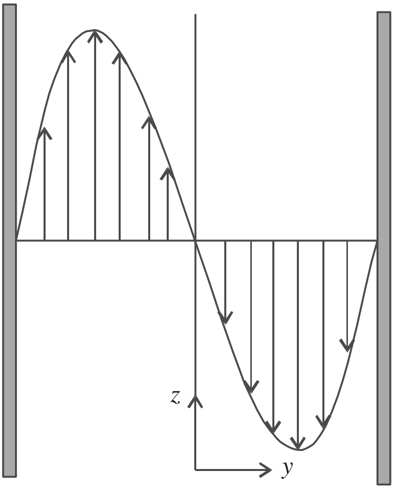
Let us define a dimensionless velocity

$$\phi = \frac{b v_z \rho_{\text{ref}}}{\mu}$$

The profile (Fig. 6.3.1-2) can be expressed as

$$\phi = \frac{1}{12} N_{\text{Gr}} (\eta^3 - \eta) \tag{6.3.1-15}$$

Fig. 6.3.1-2 Velocity profile that results from a temperature difference



where

$$N_{\mathrm{Gr}} = \text{Grashof number} = \frac{\rho_{\mathrm{ref}}{}^2 \beta_{\mathrm{ref}}\, g b^3 \Delta T}{\mu^2}$$

Using a Taylor series expansion

$$\rho = \rho_{\mathrm{ref}} - \rho_{\mathrm{ref}}\beta_{\mathrm{ref}}\,(\Delta T)$$

Thus

$$\rho_{\mathrm{ref}}\beta_{\mathrm{ref}}\,(\Delta T) = \rho_{\mathrm{ref}} - \rho = \Delta\rho$$

and

$$N_{\mathrm{Gr}} = \frac{\rho_{\mathrm{ref}}\, g b^3 \Delta\rho}{\mu^2}$$

N_{Gr} typically arises in situations with free convection.

6.3.2 The Utility of Heat Transfer Coefficients: Design of Heat Exchangers

A heat exchanger is an equipment that allows the manipulation of the temperatures of two fluid streams by transferring heat from the stream at a higher temperature to the one at a lower temperature without mixing the streams. Schematics of a typical equipment for heat exchange between fluid streams is given in Fig. 6.3.2-1.

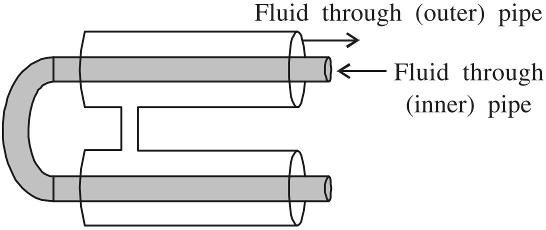


Fig. 6.3.2-1 A section of the piping arrangement in a double pipe heat exchanger. The flow shown is for the counter-current mode. The operation could also be in a co-current flow mode, where the inner pipe fluid and the outer pipe fluid move in the same direction

Let us design a heat exchanger for the following situation. The algal broth after passing through the photo-section of a bioreactor significantly increases in temperature due to heating by the sun. It needs to be cooled before it passes through the photo-section again to prevent cell death. A heat exchanger can be used to cool the broth.

The broth flows through the inner pipe of a double pipe heat exchanger, and is cooled by water flowing in the jacket. The inner pipe is made of 25 mm, schedule 40 steel pipe. The thermal conductivity of steel is 45 W m^{-1} $°C^{-1}$. Under the given conditions, the heat transfer coefficients are:

(i) Broth: 1020 W m^{-1} $°C^{-1}$
(ii) Water: 1700 W m^{-1} $°C^{-1}$

What is the overall heat transfer coefficient based on the outside area of the inner pipe? What is the rate of energy removed from the broth, if the broth at entry is at 40 °C and cooling water is available at 20 °C?

The double pipe heat exchanger can be operated in:

- Co-current (parallel) mode: Direction of hot and cold fluids are the same.
- Counter-current (anti-parallel) mode: Direction of hot and cold fluids are opposite to each other.

Figure 6.3.2-2 shows the temperature profiles of the heat exchanger when operated in both the above modes.

The desired scenario: $T_{cb} \approx T_{ha}$ i.e. cold fluid exit temperature = hot fluid entry temperature (possible to attempt with counter-current operation).

It is more practical to solve this problem using the heat-transfer coefficient approach.

$$\dot{Q} = h\,A\,(\Delta T) \qquad (6.3.2\text{-}1)$$

Fig. 6.3.2-2 Temperature profiles in a co-current and a counter-current heat exchanger

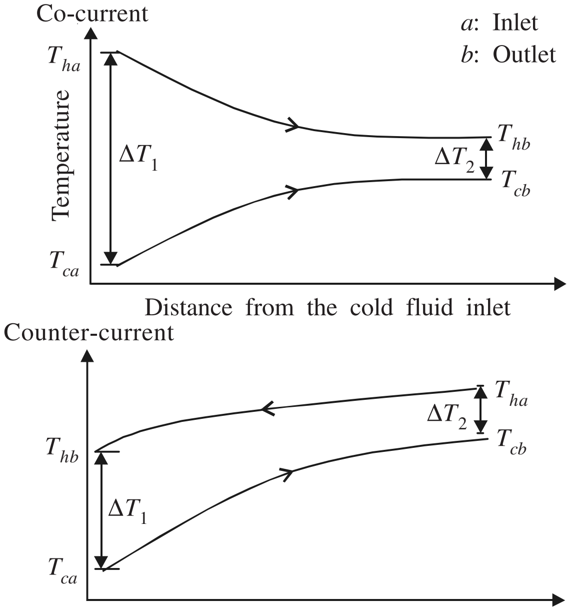
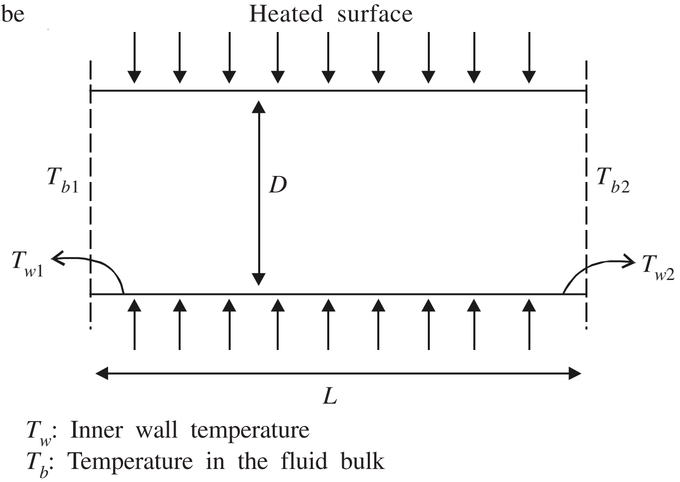


Fig. 6.3.2-3 A tube carrying a fluid with the walls heated



where $\dot{Q}$ is heat transfer rate, h is heat transfer coefficient, A is area and ΔT is temperature difference.

Note that h is not defined for a specific situation until A and ΔT are specified.

Let us consider the flow in tubes with heat being transferred through the surface (Fig. 6.3.2-3).

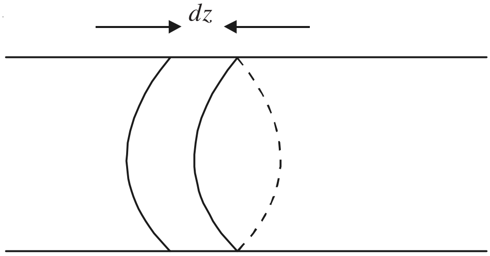


Fig. 6.3.2-4 The slice of fluid over which a force balance is performed

Three conventional definitions of the heat transfer coefficient are

$$\dot{Q} = h_1 (\pi DL)(T_{w1} - T_{b1}) \tag{6.3.2-2}$$

where h_1 is based on the initial temperature difference.

$$\dot{Q} = h_a (\pi DL)\left[\frac{(T_{w1} - T_{b1}) + (T_{w2} - T_{b2})}{2}\right] \tag{6.3.2-3}$$

where h_a is based on the arithmetic mean of the temperature difference.

$$\dot{Q} = h_{\ln} (\pi DL)\left[\frac{(T_{w1} - T_{b1}) + (T_{w2} - T_{b2})}{\ln\left\{\dfrac{T_{w1} - T_{b1}}{T_{w2} - T_{b2}}\right\}}\right] \tag{6.3.2-4}$$

where $h_{\ln}$ is based on the logarithmic mean of the temperature differences $(T_{w1} - T_{b1})_{\ln}$. $h_{\ln}$ is typically preferred because it is less dependent on $\frac{L}{D}$ than the other two coefficients. Also, if the inside wall temperature is unknown, or if the fluid properties change appreciably along the pipe, then it becomes difficult to predict the heat transfer coefficient defined earlier. Under these circumstances, a differential approach is taken wherein a force balance is performed on a slice of the fluid (Fig. 6.3.2-4).

$$dQ = h_{\text{local}} \, (\pi D dz) \, (T_w - T_b) \tag{6.3.2-5}$$

Now, let us consider the heat transfer across the heat exchanger inner pipe wall as detailed in Fig. 6.3.2-5.

The overall resistance to heat transfer (various resistances are in series)

$$R_{\text{warm fluid}} + R_{\text{wall}} + R_{\text{cold fluid}}$$

For the inner (in this case, warm) fluid

$$\frac{d\dot{Q}}{dA_i} = h_i (T_h - T_{wh}) \tag{6.3.2-6}$$

where h_i is individual heat transfer coefficient for the inner fluid.

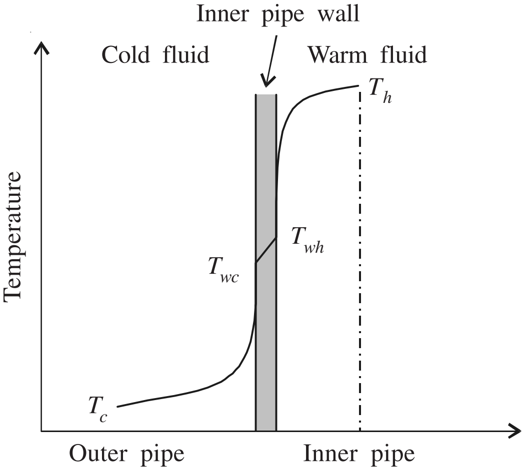


Fig. 6.3.2-5 The temperature profile across the fluids and the wall separating them in the heat exchanger

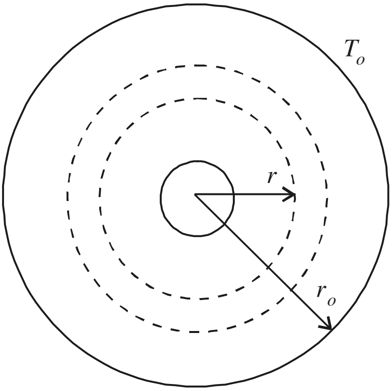


Fig. 6.3.2-6 The shell

At the wall (conduction)

$$\frac{d\dot{Q}}{dA_w} = -k\frac{dT}{dy}\bigg|_w \tag{6.3.2-7}$$

For the outer (in this case, cold) fluid

$$\frac{d\dot{Q}}{dA_o} = h_o(T_{wc} - T_c) \tag{6.3.2-8}$$

Now

$$\Delta T = T_h - T_c = (T_h - T_{wh}) + (T_{wh} - T_{wc}) + (T_{wc} - T_c) \tag{6.3.2-9}$$

Now, let us take a slight detour and consider the conduction across cylinders, to derive an expression for conductive heat rate across an annular cylinder (Fig. 6.3.2-6) when the walls are maintained at different temperatures.

$$\dot{Q} = -k\,A\frac{dT}{dr} = -k(2\pi rL)\frac{dT}{dr} \tag{6.3.2-10}$$

Upon integration

$$\int_{r_c}^{r_o} \frac{dr}{r} = \frac{2\pi Lk}{\dot{Q}} \int_{T_o}^{T_i} dT$$

$$\dot{Q} = \frac{k(2\pi L)(T_i - T_o)}{\ln\left(\dfrac{r_o}{r_i}\right)} \tag{6.3.2-11}$$

$$= \frac{k\overline{A_L}(T_i - T_o)}{r_o - r_i} \tag{6.3.2-12}$$

where

$$\overline{A_L} = \frac{(2\pi L)(r_o - r_i)}{\ln\left(\dfrac{r_o}{r_i}\right)} = 2\pi L\,\overline{r_L} \tag{6.3.2-13}$$

$\overline{A_L}$ is the logarithmic mean area, and $\overline{r_L}$ is the logarithmic mean radius, which is defined as

$$\overline{r_L} = \frac{r_o - r_i}{\ln\left(\dfrac{r_o}{r_i}\right)} \tag{6.3.2-14}$$

Using the above for the heat exchanger wall

$$\frac{d\dot{Q}}{d\overline{A_{L,w}}} = \frac{k(T_{wh} - T_{wc})}{x_w} \tag{6.3.2-15}$$

Substituting Eq. 6.3.2-15 in Eq. 6.3.2-9, we get

$$T_h - T_c = \frac{d\dot{Q}}{dA_i h_i} + \frac{d\dot{Q}}{d\overline{A_L}}\frac{x_w}{k} + \frac{d\dot{Q}}{dA_o h_o} \tag{6.3.2-16}$$

Therefore

$$\frac{d\dot{Q}}{dA_o} = \frac{T_h - T_c}{\left(\dfrac{dA_o}{dA_i}.\dfrac{1}{h_i} + \dfrac{x_w}{k}\dfrac{dA_o}{d\overline{A_L}} + \dfrac{1}{h_o}\right)} \tag{6.3.2-17}$$

We also know that

$$\frac{dA_o}{dA_i} = \frac{D_o}{D_i}$$

and

$$\frac{dA_o}{d\overline{A_L}} = \frac{D_o}{\overline{D_L}}$$

Therefore

$$\frac{d\dot{Q}}{dA_o} = \frac{T_h - T_c}{\left(\frac{D_o}{D_i}\frac{1}{h_i} + \frac{x_w}{k}\frac{D_o}{\overline{D_L}} + \frac{1}{h_o}\right)} \qquad (6.3.2\text{-}18)$$

We know that

$$\text{Flux} = \frac{\text{Driving force}}{\text{Resistance}}$$

or

$$= \text{Conductance} \times \text{Driving force}$$

Thus, the conductance

$$U_o = \frac{1}{\left(\frac{D_o}{D_i}\frac{1}{h_i}\right) + \left(\frac{D_o}{\overline{D_L}}\frac{x_w}{k}\right) + \left(\frac{1}{h_o}\right)} \qquad (6.3.2\text{-}19)$$

U_o is overall heat transfer coefficient based on the *outer* area. Similarly, it can be based on the inner area.

$$U_i = \frac{1}{\left(\frac{1}{h_i}\right) + \left(\frac{D_o}{\overline{D_L}}\frac{x_w}{k}\right) + \left(\frac{D_i}{D_o}\frac{1}{h_o}\right)} \qquad (6.3.2\text{-}20)$$

Now, let us solve the original problem.

From the schedule number and the nominal diameter given, we can find D_i, D_o using the relevant tables (as mentioned in Chapter 3). The following can be calculated

$$\overline{D_L} = \frac{D_o - D_i}{\ln\left(\frac{D_o}{D_i}\right)}$$

$$U_o = \frac{1}{\left(\frac{D_o}{D_i}\frac{1}{h_i}\right) + \left(\frac{D_o}{\overline{D_L}}\frac{x_w}{k}\right) + \left(\frac{1}{h_o}\right)}$$

and with A, $\dot{Q}$ (rate of energy removed) can be calculated.

But, how does one find h_i and h_o? Correlations are available in literature (e.g. the correlation developed by Sieder and Tate).

First, let us consider a useful non-dimensional number.

$$\text{Nusselt number, } N_{\text{Nu}} = \frac{hD}{k} \tag{6.3.2-21}$$

Thus

$$N_{\text{Nu,ln}} = \frac{h_{\text{ln}} D}{k}$$

Some approximate equations that can be used to find Nusselt number are given below.

For highly turbulent flow, i.e. for $\frac{L}{D} > 10$, $N_{\text{Re},b} > 20000$ where the subscript b represents bulk.

$$\frac{h_{\text{ln}} D}{k} = 0.026 \left(\frac{DG}{\mu_b}\right)^{0.8} \left(\frac{C_p \mu}{k}\right)^{\frac{1}{3}} \left(\frac{\mu_b}{\mu_w}\right)^{0.14} \tag{6.3.2-22}$$

where G is mass velocity = ρv, μ_b is viscosity of the bulk fluid and μ_w is viscosity of the fluid at the wall temperature.

For laminar flow

$$\frac{h_{\text{ln}} D}{k} = 1.86 \left(N_{\text{Re},b}\, N_{\text{Pr},b} \frac{D}{L}\right)^{\frac{1}{3}} \left(\frac{\mu_b}{\mu_w}\right)^{0.14} \tag{6.3.2-23}$$

A number of correlations have been developed for a variety of situations:

- Free convection
- With phase change
- Condensing liquid
- Cooling liquid
- Others

A chart similar to the Moody's chart can also be used when $N_{\text{Re},b} > 10000$. In that chart available in handbooks

$$\left(\frac{h_{\text{ln}}}{C_p G}\right)\left(\frac{C_p \mu}{k}\right)^{\frac{2}{3}} = j_h \approx \frac{f}{2}$$

which is known as the Chilton-Colburn analogy.

The properties are calculated at the mean temperature $\frac{T_b + T_w}{2}$.

6.3.3 Some Other Useful Formulations

To represent radiative heat loss from a human body, a heat transfer coefficient h_r based on the first power of temperature of the emitting and receiving bodies is used.

$$Q = h_r\,(T_s - T_w) \tag{6.3.3-1}$$

where T_s is temperature of the skin and T_w is temperature of the surrounding walls (not ambient air).

A typical value for $h_r = 5\dfrac{\text{kcal}}{\text{m}^2\,\text{h}\,°\text{C}}$.

When phase change is involved, a part of the heat flux goes toward the latent heat needed for the phase change. For example, when perspiration is considered on human skin

$$Q = \widehat{L_v}\,\dot{m} \tag{6.3.3-2}$$

where $\widehat{L_v}$ is latent heat of vaporisation per unit mass of water and $\dot{m}$ is mass rate of evaporation of water per unit surface area.

$$\dot{m} = K_{H_2O}\,\beta(\rho_{H_2O,\text{skin}} - \rho_{H_2O,\text{air}}) \tag{6.3.3-3}$$

where K_{H_2O} is mass transfer coefficient of water vapour to the surrounding air, β is fraction of skin covered by perspiration and ρ_{H_2O} is humidity (partial density of water vapour).

6.3.4 The Unsteady State Bioheat Transfer Equation

Heat transfer in tissues under unsteady state can be studied using the bioheat transfer equation developed by Pennes (1948). It is an unsteady state equation that considers conduction, metabolic heat production and the heat transfer due to blood flow to the tissue. The energy equation with the above contributions alone can be written as

$$\rho\, C_p \frac{\partial T}{\partial t} = k\nabla^2 T + \dot{Q}_m + \dot{Q}_b \tag{6.3.4-1}$$

where $\dot{Q}_m$ is the metabolic heat production rate and $\dot{Q}_b$ is the net heat generation due to blood flow.

The above equation has many applications including analysis of breast cancer.

Exercises

1. Dialysis is a treatment used to provide an artificial replacement for kidney function in people with renal failure. It works on the principle of diffusion of solutes and ultrafiltration of a fluid across a semi-permeable membrane. In an attempt to improve the procedure of dialysis, an electric field is applied in addition to a difference in concentration. Assume that only one kind of ions are present in the solution, and develop an expression for the steady state movement of ions.

2. Abnormal electrical activity in the heart, called arrhythmia, can cause cardiac arrest and consequent death. It is known that potassium chloride injected into the body can cause death. Explain the above action of potassium chloride.

3. It is reasonably well known that the transport of calcium ions across cells is important in muscle contraction. Let us consider only the transport of calcium and sodium across the cells. When the resting membrane potential of the cell membrane with reference to the sodium ions is – 105 mV, and the measured extracellular calcium ion concentration is 20 mM, estimate the intracellular calcium concentration.

4. For a simplistic estimate under certain situations, only sodium and potassium ion transports across a cell membrane are considered. The measured sodium ion concentrations are 15 mM (intracellular) and 105 mM (extracellular). The measured potassium ion concentrations are 115 mM (intracellular) and 3 mM (extracellular). With the help of the data given in the relevant example problems in the chapter, estimate the ion currents across the membrane under the above conditions (needs changes to numbers).

5. The resting potential of a myocyte is known to be – 90 mV. The intracellular and extracellular concentrations of potassium ion concentrations are found to be 150 mM and 4 mM, respectively. The intracellular and extracellular sodium ion concentrations are found to be 20 mM and 145 mM, respectively. Find the potentials by individually considering K^+ and Na^+, and thus, estimate the electrochemical driving forces in each case. If the extracellular concentrations of both the ions are increased three fold, comment on the effect of that change on the above estimated quantities.

6. For a typical neuron, under a certain set of conditions, the intracellular and extracellular Na^+ ion concentrations are 1 mM and 120 mM, respectively. At the same time, the intracellular and extracellular K^+ ion concentrations are 140 mM and 5 mM, respectively. The conductivity of Na^+ ions across the membrane is 100 pS cm^{-1} and that of K^+ is 200 pS cm^{-1}. The current flowing through the membrane reduces to 0.63 of its initial value in 100 ms. Find the current flowing initially through the membrane, and its capacitance.

7. In the Venus fly trap plant (remember the animated movie, *Ice Age 3*?), the leaves are made of two flaps. When an insect sits on the leaves, the flaps close to trap the insect inside, where it is digested by the plant. The closing of the flap is a rapid process, and many theories have been propounded to explain the same. According to one of the theories, when an insect sits on the leaf, an action potential is created. The potential difference causes the movement of H^+ and Ca^{2+} ions across the cell membrane. The diffusion of Ca^{2+} into the cell causes an influx of water into the cell (due to a decrease in a quantity called the 'water potential' of the cell). Develop an expression to relate the influx of water to the generated potential difference.

8. In *Mimosa pudica* (the touch-me-not plant), pulvinar movement, which causes the closure of the leaves, is caused by the changes in the turgor pressure. This is triggered by the efflux of potassium from the surrounding cells, followed by an efflux of water, resulting in a sudden change in the turgor pressure of the cells in the pulvinus. The membrane potential of the cells that is observed during this process at 30 °C is 130 mV compared to a resting potential of 105 mV. If the extracellular K^+ ion concentration can be assumed to be approximately constant during this process, at 5 mM, what percent of the K^+ ions are being transported out?

9. For an initial estimate, assume that the small intestine is a straight tube. Develop an expression for the steady state concentration profile of a tonic in the small intestine, if it is getting absorbed in the small intestine when the contents move forward with a velocity, v_z.

10. Pitcher pots (made of burnt clay with microscopic pores) cool water by evaporative cooling – the water in the pot diffuses out through the pores in the clay pot container, and when they evaporate from the surface into the surrounding atmosphere, they use the internal energy of water to provide the latent heat of vaporisation. The consequent reduction in the internal energy of water, reduces its temperature to a comfortable value for a pleasant drinking experience. A modification of the above, which was apparently practised by ancient Jain monks, involves closing a container (not necessarily a clay pot) filled with water with a thick cotton plug, and hanging the container, inverted. The water seeps through the cotton at larger rates compared to a regular clay surface, and cools the water inside faster through evaporative cooling. Find an expression for the time taken for the water inside to reach a desired temperature T_f. Take the water permeability across the cotton plug as k, thickness of the plug d, water viscosity μ, water density ρ, water specific heat capacity s, vessel of cylindrical cross-section of cross-sectional area A, and height h, initial water temperature T_i, latent heat of vaporisation V. (Hint: Also use Darcy's law.)

11. In a pilot-scale bioreactor, air is bubbled into a broth to provide oxygen to the aerobic organisms growing in it. The overall oxygen transfer coefficient

is determined to be 2.7×10^{-5} cm s^{-1}. Consider one bubble of diameter 5 mm which rises up the broth (predominantly water) of 1.5 m, at a velocity of 1 ms^{-1}. Estimate the amount of oxygen transferred from the bubble to the broth when the bubble rises. Also, assume equilibrium conditions. The density of air in the air bubble can be assumed to be 1.29 kg m^{-3}.

12. Perspiration is the mechanism by which human bodies lose excess heat. On a hot day, when the ambient temperature is 40 °C, assume that the thermal energy gained by the body is only by conduction through its skin. Neglect any metabolic heat generation. Estimate the needed rate of perspiration to maintain the body temperature at 37 °C. Approximate a human body to a cylinder of height 1.6 m, with a total skin area of 1.8 m^2. The average thickness of the skin is 4 mm, and its thermal conductivity is 0.3 W m^{-1} K^{-1}.

Some of the exercise problems above were suggested/formulated by T. Avaneesh, Sonia Chottani, Ramaganesh, Roopteja, Moutushi Das (1), Shruthy Suresh, Purnima Padmanabhan (2), Bhavin Chandarana, Navya, Deepanjali, Vishal (3, 4), Chaitra Prabhakar, Ashritha Durvasula, Pasupuleti Sai Shalini, K.M. Sandeep, Sattu Kishore (5), Praneet Kumat, Mandati Kumar, Amarnath M. Bhat, B. Mohan Santosh, Partha Sarathi Pati (6), Uma Maheswari, Namrata Kamat, Kiran, Kemun Khimun, Rashmi Kumari (7, 9), P. Raghavendran, P. Vivek, K. Ramasamy, M. Ashok (8, 12), Vinay Lathi, Vishnu Nair, Amit Agarwal and Pavan Kumar Allada (10).

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Appendix 1

Background on Vectors and Tensors

We know from the knowledge gained in higher secondary school that vectors are quantities that represent magnitude and direction. Thus, velocity, acceleration, force, momentum, etc., are vector quantities. We need to follow a set of rules that are different from those for numbers, to mathematically manipulate vectors. In this appendix, we will discuss some of these rules.

Consider a vector $\vec{v}$ in the rectangular coordinate system, which is intuitive. Let the components of the vector (scalars) in the three directions x, y, z be v_x, v_y, v_z and the unit vectors (of magnitude 1) in the same three directions be $\hat{\imath}_x$, $\hat{\imath}_y$, $\hat{\imath}_z$ (which are sometimes represented as $\hat{\imath}$, $\hat{\jmath}$, $\hat{k}$). We know that we can represent the vector as

$$\vec{v} = v_x\hat{\imath}_x + v_y\hat{\imath}_y + v_z\hat{\imath}_z \tag{A1-1}$$

We can express vector manipulations in compact mathematical forms by the use of $\hat{\imath}_x = \hat{\imath}_1$, $\hat{\imath}_y = \hat{\imath}_2$, $\hat{\imath}_z = \hat{\imath}_3$. Similarly, for the magnitudes too. Thus, we can write the vector as

$$\vec{v} = v_1\hat{\imath}_1 + v_2\hat{\imath}_2 + v_3\hat{\imath}_3 = \sum_{k=1}^{3} v_k\hat{\imath}_k \tag{A1-2}$$

Although we concern ourselves with a maximum of three dimensions in this book, it can be appreciated that this notation is general enough to be used even when the number of dimensions exceeds three, as in some areas of physics and mathematics.

Addition

The addition of three vectors, $\vec{u}$, $\vec{v}$ and $\vec{w}$ (can be extended to any number of vectors) can be represented in terms of its components as

$$\vec{u}+\vec{v}+\vec{w}=(u_1+v_1+w_1)\hat{\imath}_1+(u_2+v_2+w_2)\hat{\imath}_2+(u_3+v_3+w_3)\hat{\imath}_3$$

Thus, in a compact form

$$\vec{u}+\vec{v}+\vec{w}=\sum_{k=1}^{3}(u_k+v_k+w_k)\hat{\imath}_k \tag{A1-3}$$

Scalar (Dot) Product

The dot product between two vectors $\vec{u}$, $\vec{v}$, can be represented as

$$\begin{aligned}\vec{u}\cdot\vec{v}&=[u_1\hat{\imath}_1+u_2\hat{\imath}_2+u_3\hat{\imath}_3]\cdot[v_1\hat{\imath}_1+v_2\hat{\imath}_2+v_3\hat{\imath}_3]\\&=u_1v_1[\hat{\imath}_1\cdot\hat{\imath}_1]+u_1v_2[\hat{\imath}_1\cdot\hat{\imath}_2]+u_1v_3[\hat{\imath}_1\cdot\hat{\imath}_3]+u_2v_1[\hat{\imath}_2\cdot\hat{\imath}_1]+\ldots\end{aligned}$$

Let us recall that the dot product between two vectors equals the product of the magnitude of the two vectors and the cosine of the angle between them. Thus, the dot product between two unit vectors in the Cartesian coordinate system is either 1 or 0 depending on whether they are in the same direction (cos 0° = 1) or perpendicular (cos 90° = 0) to each other, respectively. Thus, the only terms that remain are

$$\vec{u}\cdot\vec{v}=u_1v_1[\hat{\imath}_1\cdot\hat{\imath}_1]+u_2v_2[\hat{\imath}_2\cdot\hat{\imath}_2]+u_3v_3[\hat{\imath}_3\cdot\hat{\imath}_3]$$

In compact notation

$$\begin{aligned}\vec{u}\cdot\vec{v}&=\left[\sum_{k=1}^{3}u_k\hat{\imath}_k\right]\cdot\left[\sum_{j=1}^{3}v_j\hat{\imath}_j\right]\\&=\sum_{k=1}^{3}\sum_{j=1}^{3}u_kv_j[\hat{\imath}_k\cdot\hat{\imath}_j]\\&=\sum_{k=1}^{3}u_kv_k\end{aligned} \tag{A1-4}$$

The Kronecker delta δ_{kj} which is defined as

$$\begin{aligned}\delta_{kj}&=1,\quad \text{if } k=j\\\delta_{kj}&=0,\quad \text{if } k\neq j\end{aligned} \tag{A1-5}$$

can be used in compact representations. For example, it can be seen by going through the indices, that

$$\hat{\imath}_k\cdot\hat{\imath}_j=\delta_{kj} \tag{A1-6}$$

Thus

$$\vec{u}\cdot\vec{v}=\sum_{k=1}^{3}\sum_{j=1}^{3}u_kv_j\delta_{kj}=\sum_{k=1}^{3}u_kv_k \tag{A1-7}$$

Vector (Cross) Product

On the same lines as above (we need to write individual components until we feel confident about the compact notation to do manipulations directly with it), the cross product between two vectors, $\vec{u}, \vec{v}$, can be represented as

$$\vec{u} \times \vec{v} = \left[\sum_{k=1}^{3} u_k \hat{\imath}_k\right] \times \left[\sum_{j=1}^{3} v_j \hat{\imath}_j\right] = \sum_{k=1}^{3} \sum_{j=1}^{3} u_k v_j [\hat{\imath}_k \times \hat{\imath}_j] \qquad \text{(A1-8)}$$

Let us recall that the cross product between two unit vectors is the product of their magnitudes and the sine of the angle between them – this could be 0 or 1 depending on whether they are in the same direction (sin 0° = 0) or perpendicular (sin 90° = 1) to each other, respectively. The direction of the resultant vector would be perpendicular to both the unit vectors, i.e. in the direction of the third coordinate; +ve or –ve direction depends on the order in which the cross product is taken. In a right-handed Cartesian coordinate system, we know that

$$[\hat{\imath}_k \times \hat{\imath}_j] = 0 \text{ if } k = j$$

and

$$[\hat{\imath}_1 \times \hat{\imath}_2] = \hat{\imath}_3; \quad [\hat{\imath}_2 \times \hat{\imath}_3] = \hat{\imath}_1; \quad [\hat{\imath}_3 \times \hat{\imath}_1] = \hat{\imath}_2 \qquad \text{(A1-9)}$$

The alternating unit tensor $\in_{kjl}$ which is defined as

$\in_{kjl} = +1$ if $jkl = 123, 231$ or 312
$\in_{kjl} = -1$ if $jkl = 321, 213$ or 132
$\in_{kjl} = 0$ if $j = k$, $k = l$ or $j = l$ (if any two indices are the same)
(A1-10)

can be used in compact notations too. For example

$$[\hat{\imath}_j \times \hat{\imath}_k] = \sum_{l=1}^{3} \in_{kjl} \hat{\imath}_l \qquad \text{(A1-11)}$$

One can expand the terms in Eq. A1-11 and check that it represents Eq. A1-9 completely, in a more compact form.

Thus

$$\vec{u} \times \vec{v} = \sum_{k=1}^{3} \sum_{j=1}^{3} u_k v_j [\hat{\imath}_k \times \hat{\imath}_j] = \sum_{l=1}^{3} u_k v_j \in_{kjl} \hat{\imath}_l \qquad \text{(A1-12)}$$

Now, using the relations in Eq. A1-9, the terms that remain in the expansion of Eq. A1-11 are

$$\vec{u} \times \vec{v} = (u_2 v_3 - u_3 v_2)\hat{\imath}_1 - (u_1 v_3 - u_3 v_1)\hat{\imath}_2 + (u_1 v_2 - u_2 v_1)\hat{\imath}_3$$

which can be conveniently evaluated as a determinant.

$$\vec{u}\times\vec{v}=\begin{vmatrix}\hat{\imath}_1 & \hat{\imath}_2 & \hat{\imath}_3\\ u_1 & u_2 & u_3\\ v_1 & v_2 & v_3\end{vmatrix} \tag{A1-13}$$

Gradient

The gradient (also known as the differential operator) is a vector. The gradient, by itself, has no physical meaning, but when it operates on a scalar or a vector, it can be physically interpreted. A gradient is represented by $\vec{\nabla}$ and is defined in the rectangular Cartesian coordinate system as

$$\vec{\nabla}=\frac{\partial}{\partial x_1}\hat{\imath}_1+\frac{\partial}{\partial x_2}\hat{\imath}_2+\frac{\partial}{\partial x_3}\hat{\imath}_3=\sum_{k=1}^{3}\frac{\partial}{\partial x_k}\hat{\imath}_k \tag{A1-14}$$

The gradient of a scalar, say density ρ becomes

$$\vec{\nabla}\rho=\sum_{k=1}^{3}\frac{\partial\rho}{\partial x_k}\hat{\imath}_k \tag{A1-15}$$

Since the gradient is a vector, it has to vectorially operate on another vector. The dot product of the gradient on a vector $\vec{v}$ is called the divergence of the vector $\vec{v}$. It is represented as

$$\vec{\nabla}\cdot\vec{v}=\left[\sum_{k=1}^{3}\frac{\partial}{\partial x_k}\hat{\imath}_k\right]\cdot\left[\sum_{j=1}^{3}v_j\hat{\imath}_j\right]=\sum_{k=1}^{3}\frac{\partial v_k}{\partial x_k} \tag{A1-16}$$

If the reader is uncomfortable at this stage with the compact notation above, it is suggested that the terms be expanded completely, so that the reader is convinced.

The gradient in cylindrical/spherical coordinate systems can be found by appropriate transformations, as given in a later sub-section of this appendix.

Laplacian Operator

The Laplacian operator ∇^2 is defined as $\vec{\nabla}\cdot\vec{\nabla}$ (note that the dot product results in a scalar). It can be represented as

$$\nabla^2=\vec{\nabla}\cdot\vec{\nabla}=\sum_{k=1}^{3}\frac{\partial^2}{\partial x_k^2} \tag{A1-17}$$

When the Laplacian operates on a scalar, say ρ

$$\nabla^2 \rho = \sum_{k=1}^{3} \frac{\partial^2 \rho}{\partial x_k^2} \tag{A1-18}$$

When the Laplacian operates on a vector, say, $\vec{v}$ in rectangular Cartesian coordinates, we get

$$\nabla^2 \vec{v} = \sum_{k=1}^{3} \frac{\partial^2 \vec{v}}{\partial x_k^2} = \sum_{k=1}^{3} \sum_{j=1}^{3} \frac{\partial^2 v_j}{\partial x_k^2} \hat{\imath}_j \tag{A1-19}$$

For curvilinear coordinates (cylindrical, spherical), appropriate transformations, as given in a later sub-section in the appendix, need to be used.

Tensors

We saw that a vector has three components. Some physical quantities such as the stress that we saw in Chapter 3, need nine components. Another quantity that also needs nine components is the dyadic product of two vectors. We will introduce another concept now called order. The second order tensor is a mathematical abstraction that can be used to represent physical quantities that need nine components. Thus, a vector can be considered a 'first order tensor' with three components.

The tensor quantities seen in Chapter 3 were the stress tensor

$$\tilde{\tau} = \begin{pmatrix} \tau_{xx} & \tau_{xy} & \tau_{xz} \\ \tau_{yx} & \tau_{yy} & \tau_{yz} \\ \tau_{zx} & \tau_{zy} & \tau_{zz} \end{pmatrix} \text{or} \begin{pmatrix} \tau_{11} & \tau_{12} & \tau_{13} \\ \tau_{21} & \tau_{22} & \tau_{23} \\ \tau_{31} & \tau_{32} & \tau_{33} \end{pmatrix} \tag{A1-20}$$

and the dyadic product of two vectors, $\vec{v}$ and $\vec{w}$ represented as

$$\vec{v}\vec{w} = \begin{pmatrix} v_x w_x & v_x w_y & v_x w_z \\ v_y w_x & v_y w_y & v_y w_z \\ v_z w_x & v_z w_y & v_z w_z \end{pmatrix} \text{or} \begin{pmatrix} v_1 w_1 & v_1 w_2 & v_1 w_3 \\ v_2 w_1 & v_2 w_2 & v_2 w_3 \\ v_3 w_1 & v_3 w_2 & v_3 w_3 \end{pmatrix} \tag{A1-21}$$

Thus, the dyadic product of unit vectors can be expressed as

$$\hat{\imath}_1 \hat{\imath}_1 = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix} \tag{A1-22}$$

$$\hat{\imath}_1\hat{\imath}_2 = \begin{pmatrix} 0 & 1 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix} \tag{A1-23}$$

$$\hat{\imath}_1\hat{\imath}_3 = \begin{pmatrix} 0 & 0 & 1 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix} \tag{A1-24}$$

and so on. These are called unit dyads.

There would be six other possible unit dyads for three dimensions: $\hat{\imath}_2\hat{\imath}_1$, $\hat{\imath}_2\hat{\imath}_2$, $\hat{\imath}_2\hat{\imath}_3$, $\hat{\imath}_3\hat{\imath}_1$, $\hat{\imath}_3\hat{\imath}_2$, $\hat{\imath}_3\hat{\imath}_3$.

Thus, the tensor $\tilde{\tau}$ can be expressed in a compact form as the sum of the products of its component with the unit dyads.

$$\tilde{\tau} = \tau_{11}\begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix} + \tau_{12}\begin{pmatrix} 0 & 1 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix} + \ldots + \tau_{33}\begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

In other words, the tensor can be expressed in a compact form as

$$\tilde{\tau} = \sum_{j=1}^{3}\sum_{k=1}^{3}(\tau_{jk})\hat{\imath}_j\hat{\imath}_k \tag{A1-25}$$

Now, let us look at the components of some operations involving tensors.

Tensor Addition of Two Tensors $\tilde{\tau}$ and $\tilde{\omega}$

$$\tilde{\tau} + \tilde{\omega} = \begin{pmatrix} \tau_{11}+\omega_{11} & \tau_{12}+\omega_{12} & \tau_{13}+\omega_{13} \\ \tau_{21}+\omega_{21} & \tau_{22}+\omega_{22} & \tau_{23}+\omega_{23} \\ \tau_{31}+\omega_{31} & \tau_{32}+\omega_{32} & \tau_{33}+\omega_{33} \end{pmatrix} \tag{A1-26}$$

$$\tilde{\tau} + \tilde{\omega} = \sum_{j=1}^{3}\sum_{k=1}^{3}(\tau_{jk} + \omega_{jk})\hat{\imath}_j\hat{\imath}_k \tag{A1-27}$$

Multiplication of a Tensor $\tilde{\tau}$ by a Scalar *s*

$$s\tilde{\tau} = \sum_{j=1}^{3}\sum_{k=1}^{3}(s\tau_{jk})\hat{\imath}_j\hat{\imath}_k \tag{A1-28}$$

If the above compact form is not clear, it will be good to write down the expansion, term wise, to see how the compact form captures the expansions. Further, some identities given later, may be needed to arrive at the final forms starting from the compact expressions of the terms involved in the operation. In this particular operation, essentially, each term in the tensor components (in the matrix), gets multiplied by the scalar *s*. We will use the compact forms from now on, and the reader who is not comfortable as yet is recommended to expand each term in terms of the tensor components and unit dyads, to understand better.

Scalar Product (Also Known as the Double Dot Product) of Two Tensors $\tilde{\tau}$ and $\tilde{\omega}$

The double dot product between two tensors results in a scalar whose value is obtained as

$$\tilde{\tau} : \tilde{\omega} = \sum_{j=1}^{3} \sum_{k=1}^{3} (\tau_{jk} \omega_{kj}) \tag{A1-29}$$

Tensor Product (Also Known as the Single Dot Product) of Two Tensors $\tilde{\tau}$ and $\tilde{\omega}$

The result of the tensor product between two tensors is a tensor. The components of the resulting tensor are obtained as follows: the *jk*th element of the resulting tensor is equal to the sum of the products of the corresponding elements of the *j*th row of $\tilde{\tau}$ and the *k*th column of $\tilde{\omega}$.

$$\tilde{\tau} \cdot \tilde{\omega} = \sum_{j=1}^{3} \sum_{k=1}^{3} \left(\sum_{l=1}^{3} \tau_{jl} \omega_{lk} \right) \hat{\imath}_j \hat{\imath}_k \tag{A1-30}$$

The dot product between a tensor $\tilde{\tau}$ and a vector $\vec{u}$ (note that a vector is a first order tensor) results in a vector whose components are obtained as follows: the *j*th element in the resulting vector is equal to the sum of the products of the corresponding elements of the *j*th row of $\tilde{\tau}$ and the (say the) column components of $\vec{u}$. In compact notation

$$\tilde{\tau} \cdot \vec{u} = \sum_{j=1}^{3} \sum_{k=1}^{3} (\tau_{jk} u_k) \hat{\imath}_j \tag{A1-31}$$

Gradient of a Vector

We had earlier discussed the gradient of a scalar. The gradient of a vector is a dyadic product between the gradient (differential operator) and the vector $\vec{v}$. Thus

$$\vec{\nabla}\vec{v} = \sum_{j=1}^{3}\sum_{k=1}^{3}\left(\frac{\partial}{\partial x_j}v_k\right)\hat{\imath}_j\hat{\imath}_k \tag{A1-32}$$

Properties and Identities

The following properties and identities involving vectors and tensors are useful. The compact forms of the various vector and tensor operations described above can be derived from the individual compact forms of the tensors and vectors involved in the operations by using some of the identities below.

$$\vec{u}\cdot\vec{v} = \vec{v}\cdot\vec{u} \tag{A1-33}$$

$$(\vec{u}\cdot\vec{v})\vec{w} \neq \vec{u}(\vec{v}\cdot\vec{w}) \tag{A1-34}$$

$$\vec{u}\cdot(\vec{v}+\vec{w}) = (\vec{u}\cdot\vec{v}) + (\vec{u}\cdot\vec{w}) \tag{A1-35}$$

The reader can recognise that the laws applicable to normal algebraic operations may not be applicable to vector operations. For example, the dot product between vectors is commutative (Eq. A1-33) and distributive (Eq. A1-35), but not associative (Eq. A1-34). On the other hand, the cross product between vectors is neither commutative (Eq. A1-36) nor associative (Eq. A1-37), but is distributive (Eq. A1-38). One can recall that addition of vectors is commutative and associative; multiplication of a vector by a scalar is commutative, associative and distributive.

$$\vec{u}\times\vec{v} \neq \vec{v}\times\vec{u} \quad \text{but} = -(\vec{v}\times\vec{u}) \tag{A1-36}$$

$$(\vec{u}\times\vec{v})\times\vec{w} \neq \vec{u}\times(\vec{v}\times\vec{w}) \tag{A1-37}$$

$$(\vec{u}+\vec{v})\times\vec{w} = (\vec{u}\times\vec{w}) + (\vec{v}\times\vec{w}) \tag{A1-38}$$

The gradient of a scalar is neither commutative nor associative, but is distributive, as shown below. Note that r and s are scalars.

$$\vec{\nabla}s \neq s\vec{\nabla} \tag{A1-39}$$

$$\vec{\nabla}(r\,s) \neq (\vec{\nabla}r)s \quad \text{but} = r(\vec{\nabla}s) + s(\vec{\nabla}r) \tag{A1-40}$$

$$\vec{\nabla}(r+s) = \vec{\nabla}r + \vec{\nabla}s \tag{A1-41}$$

The divergence of a vector is neither commutative nor associative, but is distributive, as shown below.

$$\vec{\nabla}\cdot\vec{u} \neq \vec{u}\cdot\vec{\nabla} \tag{A1-42}$$

$$\vec{\nabla} \cdot s\vec{u} \neq \vec{\nabla} s \cdot \vec{u} \tag{A1-43}$$

$$\vec{\nabla} \cdot (\vec{u} + \vec{v}) = (\vec{\nabla} \cdot \vec{u}) + (\vec{\nabla} \cdot \vec{v}) \tag{A1-44}$$

Dyadic multiplication is neither commutative nor associative, but is distributive.

$$\vec{u}\vec{v} \neq \vec{v}\vec{u} \tag{A1-45}$$

$$\vec{u} \cdot (\vec{v}\vec{w}) \neq (\vec{u}\vec{v}) \cdot \vec{w} \tag{A1-46}$$

$$\vec{u}(\vec{v} + \vec{w}) = (\vec{u}\vec{v}) + (\vec{u}\vec{w}) \tag{A1-47}$$

Identities

$$(\hat{\imath}_j\hat{\imath}_k \cdot \hat{\imath}_l) = \hat{\imath}_j\delta_{kl} \tag{A1-48}$$

$$(\hat{\imath}_j \cdot \hat{\imath}_k\hat{\imath}_l) = \delta_{jk}\hat{\imath}_l \tag{A1-49}$$

$$(\hat{\imath}_j\hat{\imath}_k \cdot \hat{\imath}_l\hat{\imath}_m) = \delta_{kl}\hat{\imath}_j\hat{\imath}_m \tag{A1-50}$$

$$(\hat{\imath}_j\hat{\imath}_k : \hat{\imath}_l\hat{\imath}_m) = \delta_{jm}\delta_{kl} \tag{A1-51}$$

$$(\vec{u}\vec{v} \cdot \vec{w}) = \vec{u}(\vec{v} \cdot \vec{w}) \tag{A1-52}$$

$$(\vec{u} \cdot \vec{v}\vec{w}) = (\vec{u} \cdot \vec{v})\vec{w} \tag{A1-53}$$

$$\vec{u} \times (\vec{v} \times \vec{w}) = \vec{v}(\vec{u} \cdot \vec{w}) - \vec{w}(\vec{u} \cdot \vec{v}) \tag{A1-54}$$

$$\vec{u} \cdot (\vec{v} \times \vec{w}) = \vec{v} \cdot (\vec{w} \times \vec{u}) \tag{A1-55}$$

$$(\vec{u}\vec{v} : \vec{w}\vec{z}) = (\vec{u} \cdot \vec{z})(\vec{v} \cdot \vec{w}) \tag{A1-56}$$

$$(\tilde{\tau} : \vec{u}\vec{v}) = (\tilde{\tau} \cdot \vec{u}) \cdot \vec{v} \tag{A1-57}$$

$$(\vec{u}\vec{v} : \tilde{\tau}) = \vec{u} \cdot (\vec{v} \cdot \tilde{\tau}) \tag{A1-58}$$

$$\vec{\nabla}(\vec{u} \cdot \vec{v}) = (\vec{u} \cdot \vec{\nabla})\vec{v} + (\vec{v} \cdot \vec{\nabla})\vec{u} + \vec{u} \times (\vec{\nabla} \times \vec{v}) + \vec{v} \times (\vec{\nabla} \times \vec{u}) \tag{A1-59}$$

$$\vec{\nabla} \cdot s\vec{u} = (\vec{\nabla} s \cdot \vec{u}) + s(\vec{\nabla} \cdot \vec{u}) \tag{A1-60}$$

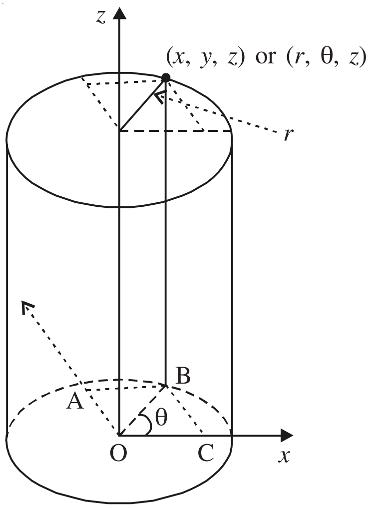
$$\vec{\nabla} \times s\vec{u} = (\vec{\nabla} s \times \vec{u}) + s(\vec{\nabla} \times \vec{u}) \tag{A1-61}$$

$$\vec{\nabla} \times \vec{\nabla} s = 0 \tag{A1-62}$$

$$\vec{\nabla} \times (\vec{u} + \vec{v}) = (\vec{\nabla} \times \vec{u}) + (\vec{\nabla} \times \vec{v}) \tag{A1-63}$$

$$\vec{\nabla} \cdot (\vec{v} \times \vec{w}) = \vec{w} \cdot (\vec{\nabla} \times \vec{v}) - \vec{v} \cdot (\vec{\nabla} \times \vec{w}) \tag{A1-64}$$

Fig. A1-1 Geometrical relationship between coordinates of a point in rectangular Cartesian coordinate and cylindrical systems



$$\vec{\nabla}\times(\vec{u}\times\vec{v})=\vec{u}(\vec{\nabla}\cdot\vec{v})-\vec{v}(\vec{\nabla}\cdot\vec{u})+(\vec{v}\cdot\vec{\nabla})\vec{u}-(\vec{u}\cdot\vec{\nabla})\vec{v} \tag{A1-65}$$

$$(\vec{\nabla}\times\vec{u})\times\vec{u}=(\vec{u}\cdot\vec{\nabla})\vec{u}-\frac{1}{2}\vec{\nabla}(\vec{u}\cdot\vec{u}) \tag{A1-66}$$

$$\vec{\nabla}\cdot\vec{\nabla}\times\vec{u}=0 \tag{A1-67}$$

$$(\vec{\nabla}\cdot\vec{v}\vec{w})=(\vec{v}\cdot\vec{\nabla}\vec{w})+\vec{w}(\vec{\nabla}\cdot\vec{v}) \tag{A1-68}$$

Transformation of Coordinates

Curvilinear coordinates such as cylindrical (r, θ, z) or spherical (r, θ, ϕ) coordinates significantly simplify the formulation of the problem equation and boundary conditions in many situations. How do we convert an equation in Cartesian coordinates to curvilinear coordinates?

Let us first consider the cylindrical system. The relationship between the coordinates of a point in Cartesian coordinate (x, y, z) and cylindrical (r, θ, z) systems is given in Fig. A1-1.

From the right triangle, OBC, it can be written that

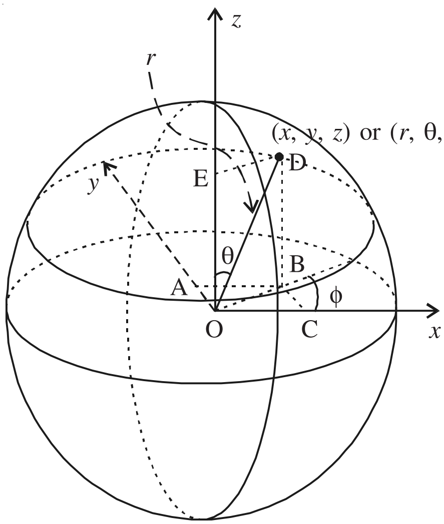
$$x = r\cos\theta \tag{A1-69}$$

$$y = r\sin\theta \tag{A1-70}$$

And, with the realisation that the z coordinate (effectively) remains the same, we can write

$$z = z \tag{A1-71}$$

Fig. A1-2 Geometrical relationship between coordinates of a point in rectangular Cartesian coordinate and spherical systems



The reverse transformation of the above, i.e. from cylindrical coordinates to rectangular Cartesian coordinates, can also be written from the geometry of the right triangle OBC or from the above three equations as

$$r = +\sqrt{x^2 + y^2} \tag{A1-72}$$

$$\theta = \tan^{-1}\left(\frac{y}{x}\right) \tag{A1-73}$$

$$z = z \tag{A1-74}$$

Now, let us do the same for the spherical coordinate system. The relationship between the coordinates of a point in Cartesian coordinate (x, y, z) and spherical (r, θ, ϕ) systems are given in Fig. A1-2. Note that θ is the angle of the radius connecting the point to the origin from the z axis, and ϕ is the angle between the projection of the same radius on the xy plane and the x-axis.

From the right triangle OED we get

$$\mathrm{ED} = r \sin\theta \quad \text{which} = \mathrm{OB} \tag{A1-75}$$

From the right triangle, OBC, we can see that

$$x = \mathrm{OB} \cos\phi$$

From Eq. A1-75, we can write the above equation as

$$x = r \sin\theta \cos\phi \tag{A1-76}$$

From the same right triangle OBC, we can also write that

$$y = r \sin\theta \sin\phi \tag{A1-77}$$

And, from the right triangle OED, we get

$$z = r\cos\theta \tag{A1-78}$$

The reverse transformation of the above, i.e. from spherical coordinates to rectangular Cartesian coordinates, can also be written from the 3D geometry, or from the above three equations as

$$r = +\sqrt{x^2 + y^2 + z^2} \tag{A1-79}$$

$$\theta = \tan^{-1}\left(\frac{\sqrt{x^2 + y^2}}{z}\right) \tag{A1-80}$$

$$\phi = \tan^{-1}\left(\frac{y}{x}\right) \tag{A1-81}$$

Next, let us see the transformation of vectors. With that we would have sufficient information to transform an equation, which is our objective.

Let us first consider the transformation to cylindrical coordinates. To understand this better, let us consider transformation of the *unit vectors* between the two coordinate systems. Once the unit vector transformation is understood, it is trivial to transform any vector since a vector is written in terms of the product of the unit vectors and components in the corresponding directions, i.e.

$$\vec{v} = v_x\hat{\imath}_x + v_y\hat{\imath}_y + v_z\hat{\imath}_z \quad \text{(in rectangular Cartesian coordinates)} \tag{A1-82}$$

$$\vec{v} = v_r\hat{\imath}_r + v_\theta\hat{\imath}_\theta + v_z\hat{\imath}_z \quad \text{(in cylindrical coordinates)} \tag{A1-83}$$

Figure A1-3 represents the unit vectors in the two coordinate systems at a point in space.

Now, let us look at the plane, z = constant, that contains the unit vectors $\hat{\imath}_r$ and $\hat{\imath}_\theta$. In other words, let us look at Fig. A1-3 from the top. The unit vectors are related as given in Fig. A1-4.

Figure A1-5 shows how the parallelogram law of addition is used for the relevant vectors in this context.

From the figure, we can write

$$\hat{\imath}_r = (\cos\theta)\hat{\imath}_x + (\sin\theta)\hat{\imath}_y \tag{A1-84}$$

If we consider the above in a 3D situation, since there is no contribution from the z direction, we can represent the unit vectors, for completeness, as

$$\hat{\imath}_r = (\cos\theta)\hat{\imath}_x + (\sin\theta)\hat{\imath}_y + (0)\hat{\imath}_z \tag{A1-85}$$

Fig. A1-3 Relationship between the unit vectors in rectangular Cartesian coordinates and in cylindrical coordinates. Note that the unit vectors in the z-direction in both the coordinate systems, although distinct in meaning, overlap each other

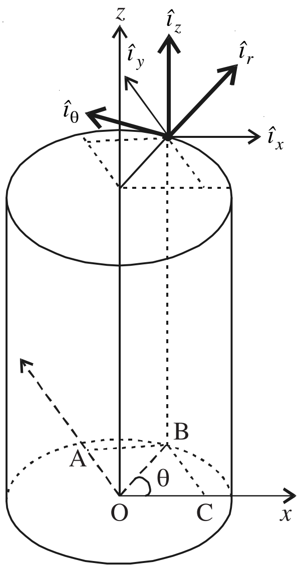


Fig. A1-4 Top view of Fig. A1-3

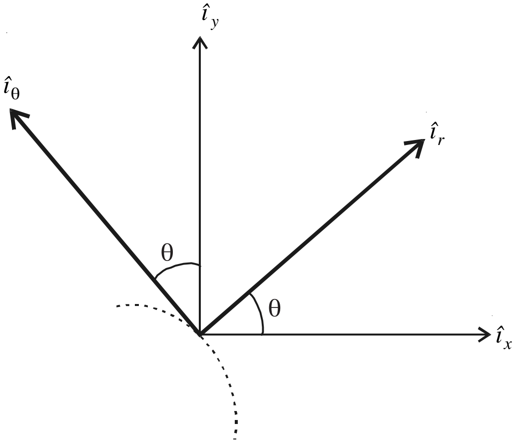
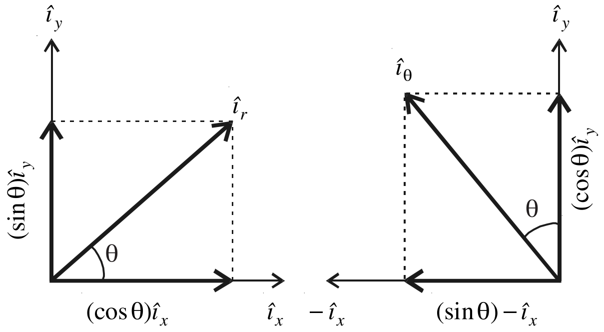


Fig. A1-5 Addition of the relevant vectors by parallelogram law



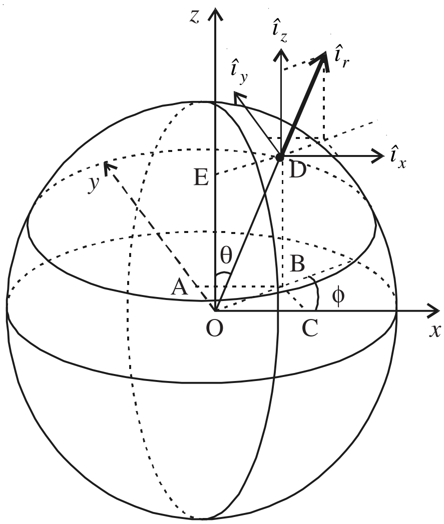


Fig. A1-6 The unit vector in the *r* direction in spherical coordinates

Similarly, we can write

$$\hat{\imath}_\theta = (-\sin\theta)\hat{\imath}_x + (\cos\theta)\hat{\imath}_y + (0)\hat{\imath}_z \qquad \text{(A1-86)}$$

And from Fig. A1-3, it is clear that the unit vectors in the *z* direction are similar, i.e.

$$\hat{\imath}_z = (0)\hat{\imath}_x + (0)\hat{\imath}_y + \hat{\imath}_z \qquad \text{(A1-87)}$$

Equations A1-85 to A1-87 provide the transformation equations to transform vectors from rectangular Cartesian to cylindrical coordinates. A similar geometrical exercise, but with the unit vectors in the cylindrical coordinates as the base, would yield the reverse transformation for vectors from cylindrical to rectangular Cartesian coordinates. The reverse transformation equations are (the reader is encouraged to work out the details of the geometry on the same lines as above)

$$\hat{\imath}_x = (\cos\theta)\hat{\imath}_r + (-\sin\theta)\hat{\imath}_\theta + (0)\hat{\imath}_z \qquad \text{(A1-88)}$$

$$\hat{\imath}_y = (\sin\theta)\hat{\imath}_r + (\cos\theta)\hat{\imath}_\theta + (0)\hat{\imath}_z \qquad \text{(A1-89)}$$

$$\hat{\imath}_z = (0)\hat{\imath}_r + (0)\hat{\imath}_\theta + (1)\hat{\imath}_z \qquad \text{(A1-90)}$$

Now, let us consider spherical coordinates. Unlike cylindrical coordinates, which by its very nature allowed us to understand the transformation by considering two effective dimensions (*z* was similar), we need to consider manipulations in three dimensions for the transformation of a vector in rectangular Cartesian coordinates to that in spherical coordinates. Let us again consider a unit vector in the *r* direction, for illustration, and then extend the same to the other two unit vectors (Fig. A1-6).

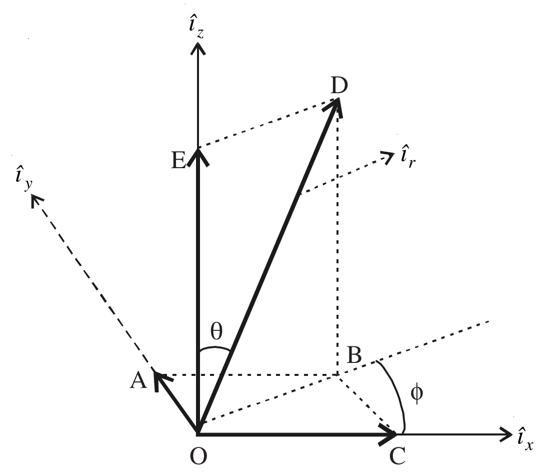


Fig. A1-7 Addition of the components in the *x*, *y* and *z* directions in three dimensions by the parallelepiped law to get $\hat{\imath}_r$

From Fig. A1-7, it can be seen that addition of the vectors $\overrightarrow{OC}$, $\overrightarrow{OA}$, $\overrightarrow{OE}$ results in $\hat{\imath}_r$, according to the parallelepiped law.

$$OC = OB \cos\phi = ED \cos\phi = (OD \sin\theta) \cos\phi$$

OD is the magnitude of the unit vector $\hat{\imath}_r$ and, thus, equals 1.

Therefore OC = (sin θ) cos ϕ and

$$\overrightarrow{OC} = (\sin\theta)\cos\phi\,\hat{\imath}_x$$

By similar trigonometric arguments

$$\overrightarrow{OA} = (\sin\theta)\sin\phi\,\hat{\imath}_y$$

$$\overrightarrow{OE} = \cos\theta\,\hat{\imath}_z$$

Thus

$$\hat{\imath}_r = (\sin\theta)\cos\phi\,\hat{\imath}_x + (\sin\theta)\sin\phi\,\hat{\imath}_y + \cos\theta\,\hat{\imath}_z \tag{A1-91}$$

By similar geometric arguments, the other two unit vectors in spherical coordinates can be written in terms of the unit vectors in the rectangular Cartesian coordinates as

$$\hat{\imath}_\theta = (\cos\theta)\cos\phi\,\hat{\imath}_x + (\cos\theta)\sin\phi\,\hat{\imath}_y + (-\sin\theta)\,\hat{\imath}_z \tag{A1-92}$$

$$\hat{\imath}_\phi = (-\sin\phi)\,\hat{\imath}_x + \cos\phi\,\hat{\imath}_y + (0)\,\hat{\imath}_z \tag{A1-93}$$

The reverse transformation from spherical coordinates to rectangular Cartesian coordinates, through similar arguments, but by taking the unit vectors in the spherical coordinates as the base, would yield

$$\hat{\imath}_x = (\sin\theta)\cos\phi\,\hat{\imath}_r + (\cos\theta)\cos\phi\,\hat{\imath}_\theta + (-\sin\phi)\,\hat{\imath}_\phi \tag{A1-94}$$

$$\hat{\imath}_y = (\sin\theta)\sin\phi\,\hat{\imath}_r + (\cos\theta)\sin\phi\,\hat{\imath}_\theta + (\cos\phi)\,\hat{\imath}_\phi \tag{A1-95}$$

$$\hat{\imath}_z = (\cos\theta)\,\hat{\imath}_r + (-\sin\theta)\,\hat{\imath}_\theta + (0)\,\hat{\imath}_\phi \tag{A1-96}$$

Let us recall that any vector can be written in terms of scalars (component magnitudes) and the unit vectors in the relevant directions as shown in Eq. A1-1 or Eq. A1-2.

So far, we have seen the transformation of position, and vectors between coordinate systems; we considered only the rectangular Cartesian, cylindrical and the spherical coordinate systems for transformation, all of which are orthogonal systems, i.e. the unit vectors in each of these systems are perpendicular to each other. For our purposes, with transformation of the derivatives, we will have enough bases to attempt transformation of the relevant equations.

To see the relevance better, let us choose to convert the equation of continuity given in Cartesian coordinates to curvilinear coordinates. First, we must write the equation in terms of its components, in which the derivatives of scalar components are present. Our general strategy for the transformation is to use the relevant expressions in the curvilinear coordinates, for the corresponding terms in the Cartesian coordinate system.

We had derived the equation of continuity in terms of rectangular (x, y, z) coordinates. To recall, in its expanded form (it is good to start with expanded forms for our strategy given below to work well), it was

$$\frac{\partial\rho}{\partial t} + \left(\frac{\partial}{\partial x}\rho v_x + \frac{\partial}{\partial y}\rho v_y + \frac{\partial}{\partial z}\rho v_z\right) = 0 \tag{A1-97}$$

To transform the coordinates, the chain rule of partial differentiation can be used.

For example, let us consider

$$v_x = f(r,\ \theta,\ z) \tag{A1-98}$$

As seen earlier, each of the cylindrical coordinates (r, θ, z) can be considered as a function of x, y, z. The actual functionality may not depend on all three, i.e. x, y and z for each one of the cylindrical coordinates. In the interest of a generalised approach which can also be applied to spherical coordinates, it will be good to consider the complete functionality now. Later, the actual functionality can be considered in detail to cancel the irrelevant terms.

Taking the partial derivative of v_x w.r.t. x at constant y, z (see Eq. A1-98 for the dependence), we can write

$$\left(\frac{\partial v_x}{\partial x}\right)_{y,z} = \left(\frac{\partial v_x}{\partial r}\right)_{\theta,z}\left(\frac{\partial r}{\partial x}\right)_{y,z} + \left(\frac{\partial v_x}{\partial \theta}\right)_{r,z}\left(\frac{\partial \theta}{\partial x}\right)_{y,z} + \left(\frac{\partial v_x}{\partial z}\right)_{r,\theta}\left(\frac{\partial z}{\partial x}\right)_{y,z} \tag{A1-99}$$

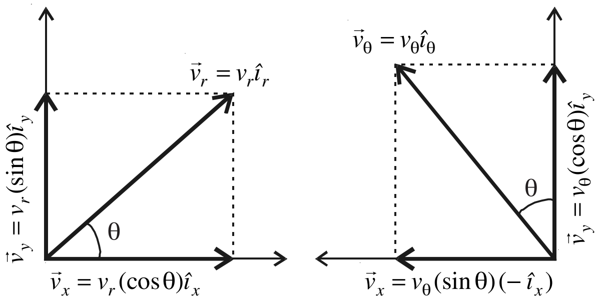


Fig. A1-8 Relationship between the vector components in rectangular Cartesian coordinate and cylindrical coordinate systems (*z* direction is irrelevant for the current argument)

Since *z* in cylindrical coordinates is independent of *x*, the last term on the RHS of the above equation is 0. Thus

$$\left(\frac{\partial v_x}{\partial x}\right)_{y,z} = \left(\frac{\partial v_x}{\partial r}\right)_{\theta,z}\left(\frac{\partial r}{\partial x}\right)_{y,z} + \left(\frac{\partial v_x}{\partial \theta}\right)_{r,z}\left(\frac{\partial \theta}{\partial x}\right)_{y,z} \qquad \text{(A1-100)}$$

Now, the above steps for v_y and v_z would yield

$$\left(\frac{\partial v_y}{\partial y}\right)_{x,z} = \left(\frac{\partial v_y}{\partial y}\right)_{\theta,z}\left(\frac{\partial r}{\partial y}\right)_{x,z} + \left(\frac{\partial v_y}{\partial \theta}\right)_{r,z}\left(\frac{\partial \theta}{\partial y}\right)_{x,z} \qquad \text{(A1-101)}$$

$$\left(\frac{\partial v_z}{\partial z}\right)_{x,y} = \left(\frac{\partial v_z}{\partial r}\right)_{\theta,z}\left(\frac{\partial r}{\partial z}\right)_{x,y} + \left(\frac{\partial v_z}{\partial \theta}\right)_{r,z}\left(\frac{\partial \theta}{\partial z}\right)_{x,y} + \left(\frac{\partial v_z}{\partial z}\right)_{r,\theta}\left(\frac{\partial z}{\partial z}\right)_{y,z}$$

As seen earlier, *r* and θ depend only on *x* and *y*, and if they are held constant, $\left(\frac{\partial r}{\partial z}\right)_{x,y} = 0$ and $\left(\frac{\partial \theta}{\partial z}\right)_{x,y} = 0$.

Therefore

$$\left(\frac{\partial v_z}{\partial z}\right)_{x,y} = \left(\frac{\partial v_z}{\partial z}\right)_{r,\theta} \qquad \text{(A1-102)}$$

Now, let us consider a vector

$$\vec{v} = v_x\hat{\imath}_x + v_y\hat{\imath}_y + v_z\hat{\imath}_z \text{ (in rectangular Cartesian coordinates)} \qquad \text{(A1-82)}$$

$$\vec{v} = v_r\hat{\imath}_r + v_\theta\hat{\imath}_\theta + v_z\hat{\imath}_z \text{ (in cylindrical coordinates)} \qquad \text{(A1-83)}$$

Extending the arguments made earlier in this section for the unit vectors, to the components of the vector $\vec{v}$, the relationships given in Fig. A1-8 can be appreciated.

From Fig. A1-8, it is clear that $\vec{v}_x$ has contributions from both $\vec{v}_r$ and $\vec{v}_\theta$ and so does $\vec{v}_y$. It can also be appreciated that the magnitudes can be expressed as

$$v_x = v_r \cos\theta - v_\theta \sin\theta \tag{A1-103}$$

$$v_y = v_r \sin\theta - v_\theta \cos\theta \tag{A1-104}$$

$$v_z = v_z \tag{A1-105}$$

Substituting Eqs. A1-103 to A1-105 in the various terms in the RHS of Eqs. A1-100 to A1-102 and differentiating, we get

$$\left(\frac{\partial v_x}{\partial r}\right)_{\theta,z} = \frac{\partial v_r}{\partial r}\cos\theta - \frac{\partial v_\theta}{\partial r}\sin\theta \tag{A1-106}$$

$$\left(\frac{\partial v_x}{\partial \theta}\right)_{r,z} = -\, v_r \sin\theta + \frac{\partial v_r}{\partial \theta}\cos\theta - v_\theta \cos\theta - \frac{\partial v_\theta}{\partial \theta}\sin\theta \tag{A1-107}$$

$$\left(\frac{\partial v_y}{\partial r}\right)_{\theta,z} = \frac{\partial v_r}{\partial r}\sin\theta + \frac{\partial v_\theta}{\partial r}\cos\theta \tag{A1-108}$$

$$\left(\frac{\partial v_y}{\partial \theta}\right)_{r,z} = v_r \cos\theta + \frac{\partial v_r}{\partial \theta}\sin\theta - v_\theta \sin\theta + \frac{\partial v_\theta}{\partial \theta}\cos\theta \tag{A1-109}$$

For the remaining terms on the RHS of A1-100 to A1-102, let us use Eqs. A1-72 to A1-73.

$$\left(\frac{\partial r}{\partial x}\right)_{y,z} = \left(\frac{\partial\left(\sqrt{x^2+y^2}\right)}{\partial x}\right)_{y,z} = \frac{1}{2}\frac{2x}{\left(\sqrt{x^2+y^2}\right)} = \frac{x}{r} = \cos\theta \tag{A1-110}$$

$$\left(\frac{\partial \theta}{\partial x}\right)_{y,z} = \left(\frac{\partial\left(\tan^{-1}\left(\frac{y}{x}\right)\right)}{\partial x}\right)_{y,z} = \frac{1}{\left(1+\left(\frac{y}{x}\right)^2\right)}\, y\left(-\frac{1}{x^2}\right) = \frac{-y}{r^2} = -\frac{\sin\theta}{r} \tag{A1-111}$$

$$\left(\frac{\partial r}{\partial y}\right)_{x,z} = \left(\frac{\partial\left(\sqrt{x^2+y^2}\right)}{\partial y}\right)_{x,z} = \frac{1}{2}\frac{2y}{\left(\sqrt{x^2+y^2}\right)} = \frac{y}{r} = \sin\theta \tag{A1-112}$$

$$\left(\frac{\partial \theta}{\partial y}\right)_{x,z} = \left(\frac{\partial\left(\tan^{-1}\left(\frac{y}{x}\right)\right)}{\partial y}\right)_{x,z} = \frac{1}{\left(1+\left(\frac{y}{x}\right)^2\right)}\left(\frac{1}{x}\right) = \frac{x}{r^2} = \frac{\cos\theta}{r} \tag{A1-113}$$

Now, we know that

$$\vec{\nabla}.\vec{v} = \left(\frac{\partial v_x}{\partial x}\right) + \left(\frac{\partial v_y}{\partial y}\right) + \left(\frac{\partial v_z}{\partial z}\right) \tag{A1-114}$$

Writing Eq. A1-114 in terms of Eqs. A1-100 to A1-102, with terms substituted from Eqs. A1-106 to A1-113, we get

$$\begin{aligned}\vec{\nabla}.\vec{v} = &\left\{\left(\frac{\partial v_r}{\partial r}\cos\theta - \frac{\partial v_\theta}{\partial r}\sin\theta\right)\cos\theta\right.\\ &\left.+\left(-v_r\sin\theta + \frac{\partial v_r}{\partial \theta}\cos\theta - v_\theta\cos\theta - \frac{\partial v_\theta}{\partial \theta}\sin\theta\right)\left(\frac{-\sin\theta}{r}\right)\right\}\\ &+\left\{\left(\frac{\partial v_r}{\partial r}\sin\theta + \frac{\partial v_\theta}{\partial r}\cos\theta\right)\sin\theta\right.\\ &\left.+\left(v_r\cos\theta + \frac{\partial v_r}{\partial \theta}\sin\theta - v_\theta\sin\theta + \frac{\partial v_\theta}{\partial \theta}\cos\theta\right)\left(\frac{\cos\theta}{r}\right)\right\}\\ &+\left\{\left(\frac{\partial v_z}{\partial z}\right)_{r,\theta}\right\}\end{aligned}$$

The RHS of the above equation, through cancellation of the +ve and –ve terms, and grouping of the relevant terms, can be written as

$$\frac{\partial v_r}{\partial r}(\cos^2\theta + \sin^2\theta) + \frac{v_r}{r}(\sin^2\theta + \cos^2\theta) + \frac{\partial v_\theta}{\partial \theta}\frac{(\sin^2\theta + \cos^2\theta)}{r} + \frac{\partial v_z}{\partial z}$$

or

$$\left(\frac{\partial v_r}{\partial r} + \frac{v_r}{r}\right) + \frac{1}{r}\frac{\partial v_\theta}{\partial \theta} + \frac{\partial v_z}{\partial z}$$

or

$$\vec{\nabla}.\vec{v} = \frac{1}{r}\frac{\partial (r\,v_r)}{\partial r} + \frac{1}{r}\frac{\partial v_\theta}{\partial \theta} + \frac{\partial v_z}{\partial z} \tag{A1-115}$$

A common error occurs with the user not realising that $\vec{\nabla}.\vec{v} \neq \frac{\partial (v_r)}{\partial r} + \frac{\partial v_\theta}{\partial \theta} + \frac{\partial v_z}{\partial z}$.

Thus, the equation of continuity in cylindrical coordinates is

$$\frac{\partial \rho}{\partial t} + \frac{1}{r}\frac{\partial (\rho\, r\, v_r)}{\partial r} + \frac{1}{r}\frac{\partial (v_\theta)}{\partial \theta} + \frac{\partial (\rho v_z)}{\partial z} = 0 \tag{A1-116}$$

To obtain an expression for $\vec{\nabla}$ in cylindrical coordinates, let us start with

$$\vec{\nabla} = \left(\frac{\partial}{\partial x}\right)\hat{\imath}_x + \left(\frac{\partial}{\partial y}\right)\hat{\imath}_y + \left(\frac{\partial}{\partial z}\right)\hat{\imath}_z$$

and write the various terms in the above equation in terms of the equivalent terms in the cylindrical coordinate system, as done in the derivation for $\vec{\nabla}.\vec{v}$. We get

$$\vec{\nabla} = \left(\frac{\partial}{\partial r}\right)\hat{\imath}_r + \frac{1}{r}\left(\frac{\partial}{\partial \theta}\right)\hat{\imath}_\theta + \left(\frac{\partial}{\partial z}\right)\hat{\imath}_z \tag{A1-117}$$

Similar derivations as above (all three dimensions would be relevant here as in the case of position), can be done for spherical coordinates with the recognition that

$$v_x = v_r \sin\theta\cos\phi + v_\theta \cos\theta\cos\phi - v_\phi \sin\phi \tag{A1-118}$$

$$v_y = v_r \sin\theta\sin\phi + v_\theta \cos\theta\sin\phi + v_\phi \cos\phi \tag{A1-119}$$

$$v_z = v_r \cos\theta - v_\theta \sin\theta \tag{A1-120}$$

and

$$v_r = v_x \sin\theta\cos\phi + v_y \sin\theta\sin\phi + v_z \cos\theta \tag{A1-121}$$

$$v_\theta = v_x \cos\theta\cos\phi + v_y \cos\theta\sin\phi - v_z \sin\theta \tag{A1-122}$$

$$v_\phi = - v_x \sin\phi + v_y \cos\phi \tag{A1-123}$$

yields the following as the equation of continuity in spherical coordinates

$$\frac{\partial \rho}{\partial t} + \frac{1}{r^2}\frac{\partial(\rho r^2 v_r)}{\partial r} + \frac{1}{r\sin\theta}\frac{\partial(\rho v_\theta \sin\theta)}{\partial \theta} + \frac{1}{r\sin\theta}\frac{\partial(\rho v_\phi)}{\partial \phi} = 0 \tag{A1-124}$$

and

$$\vec{\nabla} = \frac{\partial}{\partial r}\hat{\imath}_r + \frac{1}{r}\frac{\partial}{\partial \theta}\hat{\imath}_\theta + \frac{1}{r\sin\theta}\frac{\partial}{\partial \phi}\hat{\imath}_\phi \tag{A1-125}$$

Appendix 2

Derivation of Fick's First Law

Fick's first law in one dimension (say *x*) can be derived as follows:

Let us consider an ideal gas at a particular absolute temperature *T* and let us say that we are interested in the flux of the gas molecules across a plane, a *yz* plane, located at $z = 0$. Flux, which is the amount of a substance, or the number of molecules of the substance, transferred across a unit area perpendicular to the direction of transfer, per unit time, can be given by

$$\text{Number density} \times \text{Velocity} \tag{A2-1}$$

or

$$\frac{\text{Number of molecules}}{\text{Volume}} \times \text{Velocity}$$

or

$$\left(\frac{\text{Number}}{\text{m}^3}\right) \times \left(\frac{\text{m}}{\text{s}}\right) = \left(\frac{\text{Number}}{\text{m}^2\,\text{s}}\right)$$

Thus, the flux in the *x* direction for a population of molecules can be written as

$$J_x = N \int_0^\infty v_x f(v_x)\, dv_x \tag{A2-2}$$

where *N* is the number density function and $f\,(v_x)$ is the speed distribution function, since in a population of molecules, each molecule would have a different speed, and therefore there exists a distribution of speeds.

The Maxwell speed distribution (MSD) for an ideal gas, in one dimension is given by

$$f(v_x) = \left(\frac{m}{2\pi k_B T}\right)^{0.5} \exp\left(\frac{-m v_x^2}{2 k_B T}\right) \tag{A2-3}$$

where *m* is the mass of the molecule and k_B is the Boltzmann constant.

Equation A2-3 is obtained from the Boltzmann distribution of energies in an ideal gas at an absolute temperature T i.e.

$$f(E) = A \exp\left(\frac{-E}{RT}\right) \tag{A2-4}$$

Substitution of the MSD in Eq. A2-2 and further simplification yields

$$J_x = N\left(\frac{k_B T}{2\pi m}\right)^{0.5} \tag{A2-5}$$

In other words, from the kinetic theory of gases

$$J_x = N\frac{v_{\text{avg}}}{4} \tag{A2-6}$$

where v_{avg} is the average speed of the molecules.

Also, from the kinetic theory of gases, the mean free path of the gas molecules λ is the average distance travelled by a typical gas molecule in between two sequential collisions with other gas molecules. Let us consider two planes, parallel to the plane at $x = 0$, located at a distance of λ from the plane at $x = 0$. The x positions of the planes would be $-\lambda$ and $+\lambda$, respectively. The volume between these two planes is our system of interest, and we can do a number balance on the molecules entering and leaving the system.

Thus, the net flux in the x direction would be the flux of molecules into the system through the plane at $x = -\lambda$ and the flux of molecules exiting the system through the plane at $x = +\lambda$. Thus

$$J_{x,\text{net}} = J_{x=-\lambda} - J_{x=+\lambda} \tag{A2-7}$$

Using Eq. A2-6 in Eq. A2-7 we can write

$$J_{x,\text{net}} = N|_{x=-\lambda}\frac{v_{\text{avg}}}{4} - N|_{x=+\lambda}\frac{v_{\text{avg}}}{4} \tag{A2-8}$$

Using a Taylor expansion for N, and ignoring the second and other higher order terms in the expansion, we get

$$N|_{x=+\lambda} = N|_{x=0} + \lambda\left.\frac{dN}{dx}\right|_{x=0} \tag{A2-9}$$

$$N|_{x=-\lambda} = N|_{x=0} - \lambda\left.\frac{dN}{dx}\right|_{x=0} \tag{A2-10}$$

Substitution of Eqs. A2-10 and A2-9 in Eq. A2-8 yields

$$J_{x,\text{net}} = -2\lambda\left.\frac{dN}{dx}\right|_{x=0}\frac{v_{\text{avg}}}{4} = -\frac{1}{2}v_{\text{avg}}\,\lambda\left.\frac{dN}{dx}\right|_{x=0} \tag{A2-11}$$

In the above, we assumed that all the molecules leaving the $x = -\lambda$ plane arrive at the $x = 0$ plane. But, the thermal motion of gas molecules is completely random. Hence, an orientation average of the mean free path shows that only 2/3 of molecules leaving the $x = -\lambda$ plane will arrive at the $x = 0$ plane. Thus

$$J_{x,\,\mathrm{net}} = \frac{2}{3}\left(-\left(\frac{1}{2} v_{\mathrm{avg}}\, \lambda\right) \left.\frac{dN}{dx}\right|_{x=0} \right) = -\left(\left(\frac{1}{3} v_{\mathrm{avg}}\, \lambda\right) \left.\frac{dN}{dx}\right|_{x=0} \right)$$

Thus

$$J_{x,\,\mathrm{net}} = -D \left.\frac{dN}{dx}\right|_{x=0} \tag{A2-12}$$

which is Fick's first law with $D = \left(\frac{1}{3} v_{\mathrm{avg}}\, \lambda\right)$.

Appendix 3
Diffusivity in Concentrated Solutions

As mentioned in Chapter 2, the primary driving force for mass flux being a concentration difference is only a first approximation which works well as long as we are restricted to fluxes in a single phase (gas, liquid or solid) at dilute concentrations. The actual driving force is the difference in the chemical potential of the substance being transported.

Let us develop an expression in terms of the chemical potential gradient in one dimension (1D), z, which can easily be extended to 3D.

In terms of the chemical potential gradient, one can write the mass flux of species A as

$$J_A = -D_{AB}\frac{C_A}{RT}\frac{d\mu_A}{dz} \tag{A3-1}$$

Note that the units of chemical potential are energy per mole. From thermodynamics, we know that the chemical potential of A, μ_A, can be expressed as

$$\mu_A = \mu_A^{\#} + RT\ln(\gamma_A x_A) \tag{A3-2}$$

where $\mu_A^{\#}$ is a standard value, which is a function of temperature and pressure; γ_A is the activity coefficient, which is a function of temperature, pressure and composition; x_A is the mole fraction.

Substituting Eq. A3-2 into Eq. A3-1, and recognising that $\mu_A^{\#}$ is not a function of composition, we get

$$J_A = -D_{AB}\frac{C_A}{RT}\frac{d(RT\ln(\gamma_A x_A))}{dz} = -D_{AB}\frac{C_A}{(\gamma_A x_A)}\frac{d(\gamma_A x_A)}{dz} \tag{A3-3}$$

Differentiating using the chain rule, since γ_A is a function of composition x_A, we get

$$J_A = -D_{AB}\frac{C_A}{(\gamma_A x_A)}\left(x_A\frac{d\gamma_A}{dz}+\gamma_A\frac{dx_A}{dz}\right)$$

$$= -D_{AB}C_A\left(\frac{1}{\gamma_A}\frac{d\gamma_A}{dx_A}\frac{dx_A}{dz}+\frac{1}{x_A}\frac{dx_A}{dz}\right)$$

which can further be rearranged as

$$J_A = -D_{AB}C_A\left(\frac{1}{\gamma_A}\frac{d\gamma_A}{dx_A}+\frac{1}{x_A}\right)\frac{dx_A}{dz} \tag{A3-4}$$

The term in the brackets can be written as

$$\left(\frac{1}{\gamma_A}\frac{d\gamma_A}{dx_A}+\frac{1}{x_A}\frac{dx_A}{dx_A}\right) = (d\ln\gamma_A + d\ln x_A)$$

$$= d\ln x_A\left(\frac{d\ln\gamma_A}{d\ln x_A}+1\right)$$

$$= \frac{1}{x_A}\left(\frac{d\ln\gamma_A}{d\ln x_A}+1\right)$$

Thus, Eq. A3-4 can be written as

$$J_A = -D_{AB}C_A\frac{1}{x_A}\left(\frac{d\ln\gamma_A}{d\ln x_A}+1\right)\frac{dx_A}{dz}$$

$$= -D_{AB}\frac{1}{x_A}\left(\frac{d\ln\gamma_A}{d\ln x_A}+1\right)Cx_A\frac{dx_A}{dz}$$

or

$$J_A = -D_{AB}\left(\frac{d\ln\gamma_A}{d\ln x_A}+1\right)C\frac{dx_A}{dz} = -D_{\text{eff}}\frac{dC_A}{dz} \tag{A3-5}$$

where D_{eff} is the effective diffusivity

$$D_{\text{eff}} = D_{AB}\left(\frac{d\ln\gamma_A}{d\ln x_A}+1\right) \tag{A3-6}$$

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