NEW MATHEMATICS FOR CHEMICAL ENGINEERS

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P R E F A C E

During the past two decades, chemical engineering has been advancing so rapidly that mathematical techniques play a vital role in the profession. The engineer without an adequate mathematical knowledge will find himself incapable of doing appreciable amount of engineering work. Mathematics has beome a necessary tool for solving real life problems. An increasing number of chemical engineering undergraduates in an increasing number of universities and colleges have been taking more courses which require mathematics beyond arithematic and algebra such as process dynamics and control, kinetics and reactor design, transport phenomena, modeling and simulation, thermodynamics and unit operations. Needless to say, the graduate courses, being more advanced and more inclined to theoretical research, require a strong mathematical background.

The undergraduate courses in calculus and differential equations provide a student the essential basic training of the mathematical manipulation of the differentials and integrals, and of solving a differential equation. Very little teaching is directed to the practical application and the equally important problem of developing a differential equation to express a physical or chemical phenomenom. A course in advanced calculus or any equivalent subject which is offered by a mathematics department includes many proofs of theorems and other topics of little application. In the current professional literature, many articles deal with problems using transform, vector, and finite difference methods. The modern chemical and process industry is involved directly or indirectly with the use of digital computer which requires numerical methods of analysis. To meet all these needs, a course in chemical engineering mathematics has become necessary.

This book is the outgrowth of such a course "Mathematics for Chemical Engineer" offered by the auther in the Department of Chemical Engineering at the University of Lowell, Lowell, Massachusetts 01854. It is the result of a few revisions of a set of class notes of which a large portion has been used sucessfully in a 3-semester-hour graduate course during the past ten years. The purpose of this book is to introduce modern mathematical techniques to the formulation and solution of real life chemical engineering problems. Hence, engineering applications are emphasized more than mathematical theorems and proofs which are abundant in many mathematics textbooks. Although this book comes from the lecture notes in a graduate course, it can equally well be used as undergraduate text or as a reference for professional engineers because the only pre-requisite is calculus. It is realized that some of the material, particularly the first chapter on vector analysis and a few sections in the second and third chapters, have been covered extensively in the freshman and sophomore years of mathematics in most of the universities. However, the material is more advanced in nature. In order to help the students and professional engineers reviewing what they have learned and may have forgotten in their first two undergraduate years, it is my belief that it is advantageous to have these chapters. If the instructor feels that this material is not necessary, he may select the other useful chapters for the course. Similarly, a great deal of alternate methods have also been included in order to make this book so comprehensive that the instructor has a wider choice of material for his course. It is hoped that this book will be helpful to students, undergraduate as well as graduate, and also to professional engineers.

As mentioned above, this book, which consists of eight chapters, evolves from the lecture notes taken from several mathematics references listed at the end of the book.

Chapter 1 deals with vector analysis. The operations of vectors are described first, and then Greens' and Stokes' theorems are discussed. Finally, some engineering applications of vector analysis are illustrated.

Chapter 2 discusses ordinary differential equations. Solutions of first order equations and linear differential equations with constant and variable coefficients are described first. Next, series integration, the Frobenius method, and the Bessel function are described. Lastly, miscellaneous equations such as the Cauchy, Euler, Legendre relations are presented, and formulation of ordinary differential equations are illustrated with many examples.

Chapter 3 is concerned with differentiation and the calculus of variation. The first part of the chapter describes the technique of differentiation of composite, parametric and implicit functions, the mean value and Taylor theorems, L'Hospital and the chain rule, unconstrained and constrained optimization and also differentiation of integrals. The second part illustrates some fundamental principles of the calculus of variation, several dependent and independent variables and constraint extremals. Finally, applications of unconstrained and constrained optimization, differentiation of an integral, and the calculus of variation are illustrated by four examples.

Chapter 4 deals with partial differential equations. Classification and notation are described first. Next, the Lagrange, superposition, and the transformation methods of solution of linear first order equations, the Jacobi method for nonlinear first order equations, homogeneous and nonhomogeneous linear partial differential equations with constant and variable coefficients, and linear and nonlinear second order equations are presented. Other useful methods, such as the method of separating variables, similarity, and superposition are also included. Finally, applications of partial differential equations in chemical engineering are illustrated by three examples.

Chapter 5 treats the integral transforms. Among these, the Laplace transform is discussed in great detail. Laplace transforms of ordinary and specific functions is described. Properties of the Laplace transform and its inverse are fully discussed. Its use in solving ordinary, partial differential, finite difference, and integro-difference equations and its application in chemical engineering are described in great detail. Finally, the theory of complex variables and other integral transforms are included.

Chapter 6 presents the finite difference methods which are important topic in chemical engineering because they relate closely to the stagewise operations. In this chapter, the mathematical aspect of the difference equation is described first and then followed by its application to chemical engineering problems. In the latter part of the chapter, the application of the generating function to the solution of chemical engineering problems is introduced for the first time.

Chapter 7 demonstrates the use of matrices in the solution of complicated algebraic, differential and difference equations. In this chapter, the operations and the properties of the matrices are first described, and then their application to chemical engineering problems are discussed in detail.

The last chapter, 8, dealing with numerical methods, is essential in this computer age because the success of digital computer calculations depends to a great extent on numerical techniques. In this chapter, the solution of algebraic, transcendental, polynomial, nonlinear and simultaneous, ordinary and partial differential equations by methods such as New-Raphson, Euler, Lin-Bairstow, etc. are discussed in detail. Numerical differentiation, integration, interpolation, and the method of least squares are included. In all cases, computer programs are provided for the first time in such a chemical engineering mathematics textbook.

With pleasure I wish to express my sincere appreciation to Dr. Alfred A. Donatelli, a Research Scientist at the Kendall Company, Lexington, Massachusetts who read the entire manuscript with great care and made many valuable suggestions. I am grateful to Dr. William T. Hogan, Dean of the College of Engineering, University of Lowell for his encouragement; to Dr. Donald F. Othmer, a Distinguished Professor of Chemical Engineering at the Polytechnic Institute of New York, Brooklyn for his guidance. I am also greatly indebted to my wife, Evelyn, for her inspiration, counsel, and typing. In addition, Dr. K. W. Mao, Dean of the College of Engineering and Dr. C. J. Lee, Chairman of the Industrial Chemistry, both of the National Tsing Hua University, Hsinchu, Taiwan deserves my special thanks for granting me the position as a visiting Research Professor to teach a course from this book at a critical time in the development of this text.

Ning Hsing Chen

February, 1977

CONTENTS

CHAPTER I

VECTOR ANALYSIS

In recent years, vector analysis has been considered essential in the study of transport phenomena which are concerned with the transfer of momentum, energy and mass from one point to another in a system. These transfer equations are, in general, three dimensional and hence are long and complicated. To reduce them to meaningful and compact forms, vector analysis has been an important tool. The trend toward deriving these equations in vector form has gained attention. This chapter deals with vector operations, the various theorems governing vectors, and, lastly applications of vector analysis in engineering.

1.1 Definitions

1.1.1 Vectors and Scalars

A vector is defined as a quantity having both magnitude and direction. A quantity which has magnitude but not direction is defined as a scalar. Velocity is a vector and speed is a scalar. A vector is represented by a line with an arrow $\bar{A}$. The length of the line indicates the magnitude of the vector. The arrow point in the direction of the vector.

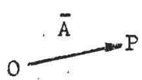


Fig.1.1-1

In Fig.1.1-1, the tail end of OP is called the origin or initial point of the vector, and the head is called the terminal point or terminus. For convenience, this vector is represented by a bar over the letter as $\bar{A}$ in this chapter.

1.1.2 Unit Vector

A vector which has unit magnitude is called a unit vector. Any vector $\bar{A}$ with magnitude $|\bar{A}| \neq 0$ has a unit vector

$$\bar{a} = \frac{\bar{A}}{|\bar{A}|} \tag{1.1-1}$$

having the same direction as $\bar{A}$.

1.1.3 Position Vectors

In three dimensional rectangular coordinates, any vector $\bar{A}$ is represented with initial point at the origin 0. Let A_x, A_y, A_z be the projections of $\bar{A}$ on the x,y,z-axes in the direction of which are the unit vectors

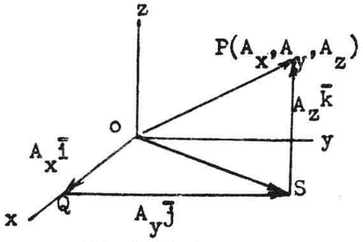


Fig.1.1-2

$\bar{i},\bar{j},\bar{k}$. Then the $A_x\bar{i}, A_y\bar{j}, A_z\bar{k}$ are component vectors of $\bar{A}$ in the x,y and z directions respectively. The sum or resultant of these component vectors is the vector $\bar{A}$

$$\bar{A} = A_x\bar{i} + A_y\bar{j} + A_z\bar{k} \qquad (1.1\text{-}2)$$

From Fig.1.1-2, it is seen that

$$\overline{OP}^2 = \overline{OS}^2 + \overline{SP}^2 \qquad (1.1\text{-}3)$$

Since

$$\overline{OS}^2 = \overline{OQ}^2 + \overline{QS}^2 \qquad (1.1.4)$$

then

$$\overline{OP}^2 = \overline{OQ}^2 + \overline{QS}^2 + \overline{SP}^2 \qquad (1.1\text{-}5)$$

or

$$|\bar{A}|^2 = A_x^2 + A_y^2 + A_z^2 \qquad (1.1\text{-}6)$$

That is, the magnitude of $\bar{A}$ is

$$|\bar{A}| = \sqrt{A_x^2 + A_y^2 + A_z^2} \qquad (1.1\text{-}7)$$

From Fig.1.1-3, it is seen that OQP is a right triangle with right angle at Q, then

$$\cos\alpha = \cos POQ = \cos(\bar{A},x) = \frac{A_x}{|\bar{A}|} \qquad (1.1\text{-}8)$$

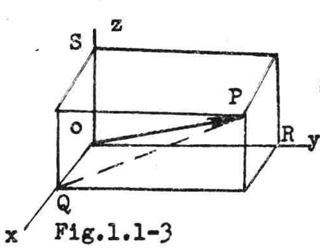


Fig.1.1-3

Similarly,

$$\cos\beta = \cos POR = \cos(\bar{A},y) = \frac{A_y}{|\bar{A}|} \qquad (1.1\text{-}9)$$

$$\cos\gamma = \cos POS = \cos(\bar{A},z) = \frac{A_z}{|\bar{A}|} \qquad (1.1\text{-}10)$$

By combining eqs.1.1-7 to 1.1-10, we obtain

$$\cos^2\alpha + \cos^2\beta + \cos^2\gamma = 1 \qquad (1.1\text{-}11)$$

in which the numbers $\cos\alpha$, $\cos\beta$, $\cos\gamma$ are called the direction cosines of $\bar{A}$.

In particular, the position vector or radius vector $\bar{r}$ from O to the point (x,y,z) is written as

$$\bar{r} = x\bar{i} + y\bar{j} + z\bar{k} \qquad (1.1.12)$$

and has magnitude

$$|\bar{r}| = (x^2 + y^2 + z^2)^{\frac{1}{2}} \qquad (1.1\text{-}13)$$

1.2 Vector Algebra

1.2.1 Vector Addition and Subtraction

When $\bar{B}$ is added to $\bar{A}$, the initial point of $\bar{B}$ should start from the terminal point of $\bar{A}$. The vector sum will be obtained by joining the initial point of the first vector $\bar{A}$ to the terminal point of the last vector as shown in Fig.1.2.1. Algebraically, it is expressed as

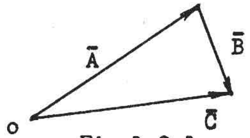


Fig.1.2-1

$$\bar{A} + \bar{B} = \bar{C} \qquad (1.2\text{-}1)$$

When several vectors are added, the resultant or sum $\bar{E}$ is obtained by joining O which is the starting point of first vector $\bar{A}$ to D, which is the terminal point of the last vector $\bar{D}$. Algebraically, it is expressed as

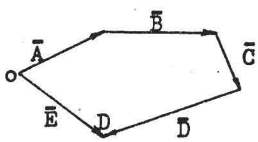


Fig.1.2-2

$$\bar{A} + \bar{B} + \bar{C} + \bar{D} = \bar{E} \qquad (1.2\text{-}2)$$

for the vectors shown in Fig.1.2-2. The vector $\bar{A} - \bar{B}$ obtained by subtracting $\bar{B}$ from $\bar{A}$ is defined as $\bar{A} + (-\bar{B})$ where $-\bar{B}$ is a vector with opposite direction but the same magnitude as $\bar{B}$. This subtraction is shown in Fig.1.2-3. Similarly, the subtraction of many vectors can be shown in Fig.1.2-4.

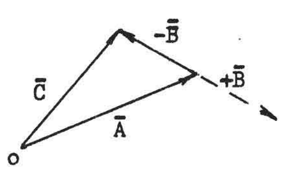


Fig.1.2-3

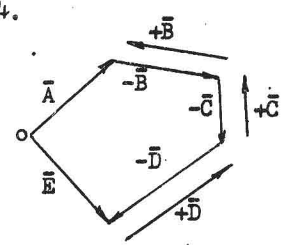


Fig.1.2-4

The following two laws are left as exercises:

$$\bar{A} + \bar{B} = \bar{B} + \bar{A} \qquad \text{commutative law} \qquad (1.2\text{-}4)$$

$$\bar{A} + (\bar{B} + \bar{C}) = (\bar{A} + \bar{B}) + \bar{C} \qquad \text{associative law} \qquad (1.2\text{-}5)$$

1.2.2 Scalar Multiplication

When a vector is multiplied by a scalar, the associative and distributive laws are valid. This means

$$(mn)\bar{A} = m(n\bar{A}) \qquad \text{associative law} \qquad (1.2\text{-}6)$$

$$(m + n)(\bar{A}) = m\bar{A} + n\bar{A} \qquad \text{distributive law} \qquad (1.2\text{-}7)$$

$$n(\bar{A} + \bar{B}) = n\bar{A} + n\bar{B} \qquad \text{distributive law} \qquad (1.2\text{-}8)$$

1.2.3 Vector Multiplication

We shall define two different types of vector multiplication: (1) scalar or dot product and (2) vector or cross product. The scalar or dot product of $\bar{A}$ and $\bar{B}$ is defined as follows:

$$\bar{A}.\bar{B} = |\bar{A}||\bar{B}| \cos\theta \qquad (1.2\text{-}9)$$

where θ is the angle between $\bar{A}$ and $\bar{B}$; see Fig.1.2-5. Thus, $\bar{A}.\bar{B}$ equals the magnitude of $\bar{A}$ times the projection of $\bar{B}$ on $\bar{A}$ or the magnitude of $\bar{B}$ times the projection of $\bar{A}$ on $\bar{B}$. It is easily verified that

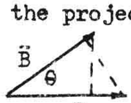


Fig.1.2-5

$$\bar{A}.\bar{B} = \bar{B}.\bar{A} \qquad (1.2\text{-}10)$$

$$(m\bar{A}).\bar{B} = m(\bar{A}.\bar{B}) \qquad (1.2\text{-}11)$$

$$\bar{A}.(\bar{B} + \bar{C}) = \bar{A}.\bar{B} + \bar{A}.\bar{C} \qquad (1.2\text{-}12)$$

It follows immediately that

$$(\bar{i}.\bar{i}) = (\bar{j}.\bar{j}) = (\bar{k}.\bar{k}) = 1 \qquad (1.2\text{-}13)$$

$$(\bar{i}.\bar{j}) = (\bar{j}.\bar{k}) = (\bar{k}.\bar{i}) = (\bar{j}.\bar{i}) = (\bar{k}.\bar{j}) = (\bar{i}.\bar{k}) = 0 \qquad (1.2\text{-}14)$$

Consequently, if

$$\bar{A} = A_x\bar{i} + A_y\bar{j} + A_z\bar{k}$$

and

$$\bar{B} = B_x\bar{i} + B_y\bar{j} + B_z\bar{k}$$

then

$$\bar{A}.\bar{B} = (A_x\bar{i} + A_y\bar{j} + A_z\bar{k}).(B_x\bar{i} + B_y\bar{j} + B_z\bar{k})$$

$$= A_xB_x + A_yB_y + A_zB_z \qquad (1.2\text{-}15)$$

Example 1.2-1: Compute the cosine of the angle between $\bar{A}$ and $\bar{B}$ if $\bar{A} = 2\bar{i} + \bar{j} + 3\bar{k}$ and $\bar{B} = -2\bar{i} + z\bar{k}$. Also find z such that $\bar{A}$ is perpendicular to $\bar{B}$.

$$\bar{A}.\bar{B} = (2\bar{i} + \bar{j} + 3\bar{k}).(-2\bar{i} + z\bar{k}) = -4 + 3z$$

From eq.1.1-7 $\bar{A} = (2^2 + 1^2 + 3^2)^{\frac{1}{2}} = 14^{\frac{1}{2}}$

$$\bar{B} = (2^2 + z^2)^{\frac{1}{2}} = (4 + z^2)^{\frac{1}{2}}$$

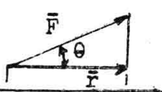
From eq.1.2-9

$$\cos(\bar{A},\bar{B}) = \frac{-4 + 3z}{[14(4 + z^2)]^{\frac{1}{2}}}$$

For $\bar{A}$ to be perpendicular to $\bar{B}$, $\cos(\bar{A},\bar{B}) = 0$ and so $z = \frac{4}{3}$

Example 1.2-2: Find the work done in moving an object along a vector $\bar{r} = 4\bar{i} + \bar{j} - 3\bar{k}$ if the applied force is $\bar{F} = 2\bar{i} - 3\bar{j} + 4\bar{k}$.

Work done = (magnitude of force in direction of $\bar{r}$).(distance)



$$= (\bar{F}\cos\theta)\,\bar{r} = \bar{F}.\bar{r}$$

$$= (2\bar{i} - 3\bar{j} + 4\bar{k}).(4\bar{i} + \bar{j} - 3\bar{k}) = 8 - 3 - 12 = -7$$

The vector or cross product of $\bar{A}$ and $\bar{B}$ is a vector whose magnitude equals the product of the magnitudes of $\bar{A}$ and $\bar{B}$ and the sine of the angle between them. The direction of the vector $\bar{C} = \bar{A} \times \bar{B}$ is perpendicular to the plane of $\bar{A}$ and $\bar{B}$ so that $\bar{A},\bar{B},\bar{C}$ form a right-handed system as shown in Fig.1.2-6 and Fig.1.2-7.

$$\bar{A} \times \bar{B} = |\bar{A}||\bar{B}|\sin\theta \qquad (1.2\text{-}16)$$

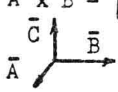


Fig.1.2-6

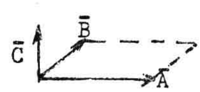


Fig.1.2-7

It is easy to verify that

$$\bar{A} \times \bar{B} = -\bar{B} \times \bar{A} \qquad (1.2\text{-}17)$$

$$\bar{A} \times (\bar{B} + \bar{C}) = \bar{A} \times \bar{B} + \bar{A} \times \bar{C} \qquad (1.2\text{-}18)$$

$$m(\bar{A} \times \bar{B}) = m\bar{A} \times \bar{B} = \bar{A} \times (m\bar{B}) = (\bar{A} \times \bar{B})m \qquad (1.2\text{-}19)$$

$$\bar{i} \times \bar{i} = \bar{j} \times \bar{j} = \bar{k} \times \bar{k} = 0 \qquad (1.2\text{-}20)$$

$$\bar{i} \times \bar{j} = \bar{k}, \qquad \bar{j} \times \bar{k} = \bar{i}, \qquad \bar{k} \times \bar{i} = \bar{j} \qquad (1.2\text{-}21)$$

If $\bar{A} = A_x\bar{i} + A_y\bar{j} + A_z\bar{k}$ and $\bar{B} = B_x\bar{i} + B_y\bar{j} + B_z\bar{k}$,

then $\bar{A} \times \bar{B} = (A_x\bar{i} + A_y\bar{j} + A_z\bar{k}) \times (B_x\bar{i} + B_y\bar{j} + B_z\bar{k})$

$$= (A_yB_z - A_zB_y)\bar{i} + (A_zB_x - A_xB_z)\bar{j} + (A_xB_y - A_yB_x)\bar{k}$$