Open-Ended Problems: A Future Chemical Engineering Education Approach. J. Patrick Abulencia and Louis Theodore.

12

Transport Phenomena

This chapter is concerned with process transport phenomena. As with all the chapters in Part II, there are several sections: overview, several technical topics, illustrative open-ended problems, and open-ended problems. The purpose of the first section is to introduce the reader to the subject of transport phenomena. As one might suppose, a comprehensive treatment is not provided although numerous references are included. The second section contains three open-ended problems; the authors' solution (there may be other solutions) are also provided. The third (and final) section contains 31 problems; *no* solutions are provided here.

12.1 Overview

This overview section is concerned—as can be noted from its title—with transport phenomena. As one might suppose, it was not possible to address all topics directly or indirectly related to transport phenomena. However, additional details may be obtained from either the references provided at the end of this Overview section and/or at the end of the chapter.

Note: Those readers already familiar with the details associated with this subject may choose to bypass this Overview.

Transport phenomena deals with the transfer of certain quantities (momentum, energy, and mass) from one point in a system to another. Three basic transport mechanisms are involved in a process. They are:

1. Radiation
2. Convection
3. Molecular diffusion.

The first mechanism, radiative transfer, arises due to wave motion and is not considered, since it may be justifiably neglected in most engineering applications. Convective transfer occurs simply due to *bulk motion*. Molecular diffusion is defined as the transport mechanism arising due to *gradients*. For example, momentum is transferred in the presence of a *velocity* gradient; energy in the form of heat is transferred due to a *temperature* gradient and mass is transferred in the presence of a *concentration* gradient. These molecular diffusion effects are described by *phenomenological* laws. These laws have been defined as mathematical models which happen to be obeyed within experimental precision by most media. Each of the laws described below reduces to the product of an appropriate transport coefficient and a gradient.

1. Newton's second law serves to define the viscosity—the transport coefficient for momentum transfer.
2. Fourier's law defines the thermal conductivity—the transport coefficient for heat transfer.
3. Fick's law serves to define the diffusivity—the transport coefficient for mass transfer.

The aforementioned transport coefficient is almost always determined by experiment, although it can be predicted theoretically from knowledge at the molecular level. The methods of evaluating and correlating these coefficients is not presented. Instead, the reader is referred to any standard text on physical properties for this information.

The remaining sections of this chapter are concerned with

1. Development of Equations
2. The Transport Equations
3. Boundary and Initial Conditions
4. Solution of Equations

5. Analogies.

It should be noted that the bulk of the material to follow has been drawn from the work of Theodore [1].

12.2 Development of Equations

Much of the materials in this section was presented in Chapter 3, Momentum, energy and mass are all conserved. As such, each quantity obeys the conservation law within a system.

$$\left\{\begin{matrix} quantity \\ into \\ system \end{matrix}\right\} - \left\{\begin{matrix} quantity \\ out\ of \\ system \end{matrix}\right\} + \left\{\begin{matrix} quantity \\ generated \\ in\ system \end{matrix}\right\} = \left\{\begin{matrix} quantity \\ accumulated \\ in\ system \end{matrix}\right\} \quad (12.1)$$

This equation may also be written on a *time* rate basis:

$$\left\{\begin{matrix} rate\ of \\ quantity \\ into \\ system \end{matrix}\right\} - \left\{\begin{matrix} rate\ of \\ quantity \\ out\ of \\ system \end{matrix}\right\} + \left\{\begin{matrix} rate\ of \\ quantity \\ generated \\ in\ system \end{matrix}\right\} = \left\{\begin{matrix} rate\ of \\ quantity \\ accumulated \\ in\ system \end{matrix}\right\} \quad (12.2)$$

The conservation law may be applied at the macroscopic, microscopic or molecular level. One can best illustrate the differences in these methods with an example. Consider a system in which a fluid is flowing through a cylindrical tube (see Figure 12.1). Define the system as the fluid contained within the tube between points 1 and 2 at any time. If one is interested in determining changes occurring at the inlet and outlet of the system, the conservation law is applied on a "macroscopic" level to the entire system. The resultant equation describes the overall changes occurring *to* the system without regard for internal variations *within* the system. This approach is usually applied in the Unit Operations (or its equivalent) courses. The microscopic approach is employed when detailed information concerning the behavior *within* the system is required, and this is often requested of and provided by the engineer. The conservation is then applied to a *differential* element within the system which is large compared to an individual molecule, but small compared to the entire system. The resultant equation

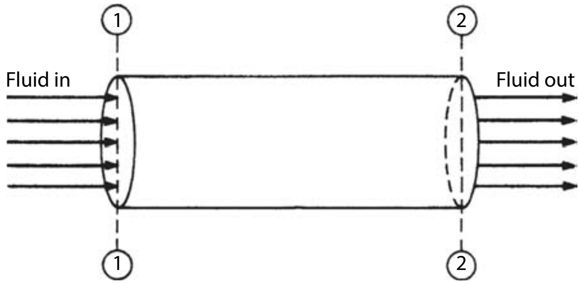

Figure 12.1 Pipe flow

is then expanded, via integration, to describe the behavior of the entire system. This is defined as the *transport phenomena* or *microscopic approach*. The molecular approach involves the application of the conservation law to individual molecules. This leads to a study of statistical and quantum mechanics—both of which are beyond the scope of this text. In any case, the description of individual matter at the molecular level is of little value to the engineer. However, the statistical averaging of molecular quantities in either a differential or finite element within a system leads to a more meaningful description of the behavior of a system.

Traditionally, the applied mathematician has developed the differential equations describing the detailed behavior of systems by applying the appropriate conservation law to a differential element or shell within the system. Equations were derived with each new application. The engineer later removed the need for these tedious and error-prone derivations by developing a general set of equations that could be used to describe systems. These are referred to as the *transport equations*. Since they are so general, they may be used rather indiscriminately to describe the infinite variety of specific problems confronting engineers. Needless to say, these transport equations have proven to be an invaluable asset in describing the behavior of many systems, operations and processes.

A complete description of the transport process requires certain additional information. The pressure, temperature, and composition dependence of viscosity, thermal conductivity, and diffusivity, must be made available from thermodynamics data. Chemical reaction systems require kinetic data.

12.3 The Transport Equations

The aforementioned transport equations are available in the literature [1,2], the details of which are significantly beyond the purpose and scope of this text. Theodore [1] developed the equations in vector form and then expanded them into the following coordinate system:

1. rectangular (Cartesian);
2. cylindrical; and
3. spherical.

Theodore's development included material concerned with the continuity, momentum transfer, energy transfer in solids, energy transfer, mass transfer in solids, and the mass transfer equations. The classic work of Bird, et al. [2] provides additional and a more expansive treatment of this subject.

12.4 Boundary and Initial Conditions

In order to solve the differential transport equation(s) so that one may obtain a complete description of the pressure, temperature, composition, etc., of a system, it is necessary to specify boundary and/or initial conditions (BC/IC) for the system. This information arises from a description of the problem or the physical situation. The number of boundary conditions (BC) that must be specified is the sum of the highest order derivative for each independent position variable appearing in the differential equation. A value specified at the boundary of the system is one type of boundary condition. The number of initial conditions (IC) that must be specified is the highest order time derivative appearing in the differential equations. This condition is used only if time is a variable. The value of the solution at time equal to zero constitutes an IC.

For example, the equation

$$\frac{d^2 v_y}{dz^2} = 0 \tag{12.3}$$

requires two BC. The equation

$$\frac{dT}{dt} = 0; \qquad t = \text{time} \tag{12.4}$$

requires one IC. And finally, the equation

$$\frac{\partial c_A}{\partial t} = D\frac{\partial^2 c_A}{\partial y^2} \tag{12.5}$$

requires one IC and two BC.

12.5 Solution of Equations

This section is introduced by outlining the general procedure that engineers should follow in solving problems in transport phenomena. The procedure is as follows.

1. Draw a line diagram representing the physical system.
2. List all pertinent variables and dimensions on the diagram.
3. Select the most convenient coordinate system.
4. Obtain the mathematical equations (in the chosen coordinates) describing the behavior of the system. This information can be "extracted" from the transport equations.
5. Specify the BC/IC.
6. Solve the equations.
7. Check to see if the solution satisfies *both* the differential equation and the BC/IC

As stated earlier, combining the conservation and phenomenological laws leads to a set of partial differential equations that can usually be solved subject to the system's BC/IC. In principle, this approach leads to a complete solution. In practice, two major difficulties may arise:

1. There is insufficient knowledge of the transport coefficients appearing in the equations.
2. The complexity of the differential equation and the accompanying BC/IC prohibits solution.

The reader is referred to other texts dealing exclusively with item (1). Information (data) on the coefficients is general available. One can then focus attention on item (2). These solutions may be obtained by:

1. Intuition
2. Graphical methods
3. Analytical methods
4. Analog methods
5. Numerical methods.

12.6 Analogies

There are certain common principles and laws that apply to the transport processes. Because of this, many similarities and analogies exist between the transport mechanisms discussed in the preceding sections; these are outlined and discussed in the present section.

Four common subject areas are discussed below. These include:

1. Conservation law
2. Phenomenological law
3. Units of molecular diffusion coefficient
4. Ratio of molecular diffusion coefficients

Details of each follows

1. *Conservation law*. Each of the equations describing the transfer of momentum, energy, and mass are developed by application of the conservation law on a rate basis to momentum, energy, and mass, respectively. The general form of the equation is

$$\begin{aligned}
&\left\{\begin{matrix}\textit{rate of property}\\ \textit{into system}\\ \textit{by molecular}\\ \textit{diffusion}\end{matrix}\right\} - \left\{\begin{matrix}\textit{rate of property}\\ \textit{out of system}\\ \textit{by molecular}\\ \textit{diffusion}\end{matrix}\right\}\\
&\qquad\qquad \downarrow\downarrow\downarrow\downarrow\downarrow\downarrow\downarrow\\
&\qquad\qquad \text{Gradients}\\
&+\left\{\begin{matrix}\textit{rate of property}\\ \textit{into system}\\ \textit{by convection}\end{matrix}\right\} - \left\{\begin{matrix}\textit{rate of property}\\ \textit{out of system}\\ \textit{by convection}\end{matrix}\right\}\\
&\qquad\qquad \downarrow\downarrow\downarrow\downarrow\downarrow\downarrow\downarrow\\
&\qquad\qquad \text{Bulk Flow}\\
&+\left\{\begin{matrix}\textit{external forces}\\ \textit{or}\\ \textit{rate of generation}\\ \textit{of property}\\ \textit{in system}\end{matrix}\right\} = \left\{\begin{matrix}\textit{rate of accumulation}\\ \textit{of property}\\ \textit{in system}\end{matrix}\right\}\\
&\quad \underset{\text{Source}}{\downarrow\downarrow\downarrow\downarrow\downarrow\downarrow\downarrow} \qquad \underset{\text{Inventory}}{\downarrow\downarrow\downarrow\downarrow\downarrow\downarrow\downarrow}
\end{aligned} \tag{12.6}$$

2. *Phenomenological law*. The laws governing the molecular diffusion of momentum, energy, and mass were developed

by Newton, Fourier, and Fick, respectively. These phenomenological laws express the corresponding fluxes for momentum, energy, and mass in terms of measurable quantities, i.e.,

$$\begin{Bmatrix} molecular \\ diffusion \\ flux \end{Bmatrix} = -\begin{Bmatrix} transport \\ coefficient \end{Bmatrix} \times \{\text{gradient}\} \tag{12.7}$$

or more specifically,

$$\tau_{zy} = -\frac{\mu}{g_c}\frac{dv_y}{dz}; \quad \text{Newton's Law} \tag{12.8}$$

$$q_z = -k\frac{dT}{dz}; \quad \text{Fourier's Law} \tag{12.9}$$

$$J_{A_z} = -D_{AB}\frac{dc_A}{dz}; \quad \text{Fick's Law} \tag{12.10}$$

with the standard notation employed in the transport field [1,2].

3. *Units of molecular diffusion coefficient.* The molecular diffusion for momentum, energy, and mass are defined

$$v = -\frac{\mu}{\rho}; \quad \text{kinematic viscosity, momentum} \tag{12.11}$$

$$a^2 = \frac{k}{\rho C_p}; \quad \text{thermal diffusivity, energy} \tag{12.12}$$

$$D_{AB} = D_{AB}; \quad \text{diffusion coefficient, mass} \tag{12.13}$$

A dimensionless analysis of these three coefficients produces an interesting result. The units of v, a^2, and D_{AB} are the same and given in ft^2/s (English units).

4. *Ratio of molecular diffusion coefficients*. The ratio of the molecular diffusion coefficients can play an important role in the analysis of a system undergoing the simultaneous transfer of any combination of momentum, energy, and/or mass. It is a measure of the relative magnitude of these effects. The three coefficients corresponding to momentum, energy, and mass previously have been defined as v, a^2, and D_{AB}, respectively. Three dimensionless ratios can be generated from these coefficients.

   a. Ratio of momentum to energy; i.e.,

$$\frac{v}{a^2} = \frac{\mu / \rho}{k / \rho C_p} \tag{12.14}$$

   This may be written as

$$\frac{\mu C_p}{k} \tag{12.15}$$

   and is defined as the Prandtl number. It finds application in fluid flow and heat transfer processes.

   b. Ratio of momentum to mass; i.e.,

$$\frac{v}{D_{AB}} \tag{12.16}$$

   or

$$\frac{\mu}{\rho D_{AB}} \tag{12.17}$$

   This term is defined as the Schmidt number and finds application in systems undergoing momentum and mass transfer.

   c. Ratio of energy to mass; i.e.,

$$\frac{a^2}{D_{AB}} = \frac{k / \rho C_p}{D_{AB}} \tag{12.18}$$

or

$$\frac{k}{\rho C_p D_{AB}} \tag{12.19}$$

This term is defined as the Lewis number. It finds application in heat and mass transfer operations.

12.7 Illustrative Open-Ended Problems

This and the last section provide open-ended problems. However, solutions *are* provided for the three problems in this section in order for the reader to hopefully obtain a better understanding of these problems which differ from the traditional problems/illustrative examples. The first problem is relatively straightforward while the third (and last problem) is somewhat more difficult and/or complex. Note that solutions are not provided for the 31 open-ended problems in the next section.

Problem 1: Describe the differences between the macroscopic, microscopic, and molecular approaches (as they apply to the conservation laws) from a technical perspective.

Solution: Refer to the development provided earlier in the Development of Equations section.

Problem 2: Outline the general procedure that chemical engineers should follow in solving problems in transport phenomena.

Solution: Solutions can be obtained almost immediately by inspection or intuition for a few of these examples. However, the majority of the differential equations encountered are solved by well-known standard analytical methods. These include:

1. Separation of variables
2. Fourier series
3. Bessel functions
4. Laplace transforms
5. Error functions.

Complet programs now permits solution to some of the more formidable problems. The more complex equations, encountered in practice, can be solved by numerical methods with a computer.

The reader is referred to the Solution of Equations section for additional details see Chapter 2.

Problem 3: A moving fluid enters the reaction zone of a tubular reactor given at concentration c_{A_0} and undergoes chemical reaction. Obtain the steady-state equations describing the concentration in the reaction zone if the flow is either laminar or plug. Assume various reaction mechanisms in generating the solutions. Do not neglect diffusion effects [1].

Solution: The problem is solved using cylindrical coordinates. Based on the problem statement

$$c_A = c_A(\mathrm{r,z}), \quad \text{laminar flow}$$

$$c_A = c_A(\mathrm{z}), \quad \text{plug flow}$$

and

$$v_r = 0$$
$$v_\phi = 0$$
$$v_z = 2v_z\left[1-\left(\frac{r}{a}\right)^2\right], \text{ laminar flow}$$
$$v_z = v_z, \quad \text{plug flow}$$

The partial differential equation describing this system for a *first order* reaction is given by

$$v_z\frac{\partial c_A}{\partial z} = D_{AB}\left[\frac{1}{r}\frac{\partial}{\partial r}\left(r\frac{\partial c_A}{\partial r}\right)+\frac{\partial^2 c_A}{\partial z^2}\right]-k_A c_A$$

For laminar flow, this equation becomes

$$\left(2\ v_z\right)\left[1-\left(\frac{r}{a}\right)^2\right]\frac{\partial c_A}{\partial z} = D_{AB}\left[\frac{1}{r}\frac{\partial}{\partial r}\left(r\frac{\partial c_A}{\partial r}\right)+\frac{\partial^2 c_A}{\partial z^2}\right]-k_A c_A$$

For plug flow,

$$v_z \frac{\partial c_A}{\partial z} = D_{AB} \frac{\partial^2 c_A}{\partial z^2} - k_A c_A$$

One can obtain the concentration profile in the reactor for laminar and plug flow. Neglecting axial and radial diffusion leads to

$$2v_z \left[1 - \left(\frac{r}{a}\right)^2\right] \frac{\partial c_A}{\partial z} = -k_A c_A$$

for laminar flow. This many now be rewritten as

$$2v_z \left[1 - \left(\frac{r}{a}\right)^2\right] \frac{dc_A}{dz} = -k_A c_A$$

The BC for this problem is

$$c_A = c_{A_0} \qquad \text{at} \qquad z = 0$$

The solution to the above equation is

$$c_A = c_{A_0} e^{-k_A z / 2v_z \left[1-(r/a)^2\right]}$$

This approach may be applied to reactions of other/different orders.

12.8 Open-Ended Problems

This last Section of the chapter contains open-ended problems as they relate to transport phenomena. No detailed and/or specific solution is provided; that task is left to the reader, noting that each problem has either a unique solution or a number of solutions or (in some cases) no solution at all. These are characteristics of open-ended problems described earlier.

There are comments associated with some, but not all, of the problems. The comments are included to assist the reader while attempting to solve the problems. However, it is recommended that the solution to each problem should initially be attempted *without* the assistance of the comments.

There are 31 open-ended problems in this section. As stated above, if difficulty is encountered in solving any particular problem, the reader should next refer to the comment, if any is provided with the problem. The reader should also note that the more difficult problems are generally located at or near the end of the section.

1. Discuss the recent advances in transport phenomena education.
   Comment: Refer to the literature for details [2].
2. Describe the early history associated with transport phenomena education.
   Comment: Refer to the literature for details [2].
3. Describe the differences between the macroscopic, microscopic, and molecular approaches from a layman's perspective.
4. Select a refereed, published transport phenomena article from the literature and provide a review.
5. Develop an original problem that would be suitable as an illustrative example in a book on transport phenomena.
6. Prepare a list of the various books that have been written on transport phenomena. Select the three best and justify your answer. Also select the three weakest books and, once again, justify your answer.
7. Provide in layman terms, the Boltzmann equation describing the kinetic theory of gases.
8. Describe and discuss the limitations associated with Boltzmann's kinetic theory of gases.
9. Attempt to improve on Boltzmann's kinetic theory of gases.
10. Describe Newton's Law of viscosity in layman terms.
11. Describe Fourier's Law in layman terms.
12. Describe Fick's Law in layman terms.
13. Discuss the differences between macroscopic and microscopic coefficients.
14. Describe the various classes of polymeric liquids. Also discuss the differences.
15. Describe the various velocity distributions that can arise for flowing fluids in conduits.

16. Discuss the differences between free and forced convection at the microscopic level.
17. Describe the complications that arise in describing multicomponent systems at the microscopic level.
18. Describe the problems associated with applying the microscopic approach to turbulent flow systems.
19. Discuss the molecular theory of predicting the viscosity of both liquids and gases.
20. Discuss the molecular theory of predicting the thermal conductivity of solids, liquids and gases.
21. Discuss the molecular theory of predicting the diffusivities of liquids, colloidal suspensions and gases.
22. Energy is being absorbed in a long solid cylinder of radius a. The temperature at the outer surface of the cylinder is maintained at a constant value T_0. Calculate the temperature profile in the solid at steady-state conditions. Assume the energy generation term A is a
    - linear,
    - quadratic, and
    - cubic

    function of the temperature. Comment on the results.
23. A long hollow *cylinder* has its inner and outer surfaces maintained at constant temperatures. Calculate the temperature profile in the solid section of the cylinder and determine the flux at both surfaces for different temperatures. Comment on the results. Assume steady-state conditions.
24. A component is reacting uniformly in a batch reactor of arbitrary shape. Obtain the concentration as a function of position and time for various reaction mechanisms if the initial concentration is everywhere constant. Assume no mass transfer across the surface of the solid.
25. An incompressible fluid enters the reaction zone of an insulated tubular (cylindrical) reactor at temperature T_0. The chemical reaction occurring in the zone causes a rate of energy per unit volume to be liberated. Obtain the steady-state equation describing the temperature in the reactor zone if the flow is laminar and the rate of energy generation is a:
    - linear
    - parabolic
    - cubic

function of temperature. Neglect axial diffusion. Also comment on the results.
Comment: Refer to the literature [3].

26. Two different viscosity fluids are contained between the region bounded by two infinite parallel horizontal plates separated by a finite distance. The volumes occupied by each fluid are equal. The upper plate is moving with a velocity that varies with time. Set up the describing equation(s) and calculate the velocity profile of both fluids for different velocity variations.
27. Consider an insulated cylindrical copper rod. If the rod is initially at a constant temperature and the ends of the rod are maintained at a temperature that varies with time, provide an equation that describes the temperature (profile) in the rod as a function of both position and time.
28. Refer to the previous problem. Calculate the temperature profile for different temperature variations.
29. Some have argued (including the senior – in terms of age – author of this book) that transport phenomena has outlived its usefulness for the chemical engineer. Comment on this statement.
30. Prepare a detailed review of the second edition of the Bird, et al. book.
31. Prepare a detailed review that highlights the differences between the first [4] and second [2] editions of the Bird, et al books.

References

1. L. Theodore, *Transport Phenomena for Engineers*, Theodore Tutorials, East Williston, NY, originally published by International Textbook CO., Scranton, PA, 1971.
2. R. Byrd, W. Stewart, and Lightfoot, *Transport Phenomena*, 2nd edition, John Wiley & Sons, Hoboken, NJ, 2002.
3. L. Theodore, *Heat Transfer for the Practicing Engineer*, John Wiley & Sons, Hoboken, NJ, 2011.
4. R. Byrd, W. Stewart, and Lightfoot, *Transport Phenomena*, John Wiley & Sons, Hoboken, NJ, 1960.