

# MODELING AND SIMULATION IN CHEMICAL ENGINEERING

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# Course Objective

- Identify the terms involved in inventory rate equation of mass, energy and momentum
- Recall the basic concepts involved in modeling and simulation
- Apply conservation of mass, momentum and energy equations to engineering problems.
- Develop model equations for chemical engineering systems
- Solve the model equations and chemical engineering problems using numerical techniques

# Introduction to Process Modeling and Simulation

- ❑ Process simulation is a successful tool for design, optimization and control of chemical processes
- ❑ Use of simulation expanded due to availability of high speed computers and software packages
- ❑ Availability of solution techniques further broadened the use of simulation

# Introduction to Process Modeling and Simulation

## Skills Required

- ❑ Sound understanding of engineering fundamentals (physical system & mechanisms).
- ❑ Process cannot be viewed as a black box!
- ❑ Modeling skills (sound mathematical relations).
- ❑ Computational skills (proper solution technique, software package, computer, etc.)

# What does “Model” mean?

- ❑ Representation of a physical system by mathematical equations
- ❑ Models at their best are no more than approximation of the real process
- ❑ Equations are based on fundamental laws of physics (conservation principle, transport phenomena, thermodynamics and chemical reaction kinetics).

# What does “Simulation” mean?

- ❑ Solving the model equations analytically or numerically.
- ❑ **Modeling & Simulation are valuable tools:** safer and cheaper to perform tests on the model using computer simulations rather than carrying repetitive experimentations and observations on the real system.

# System

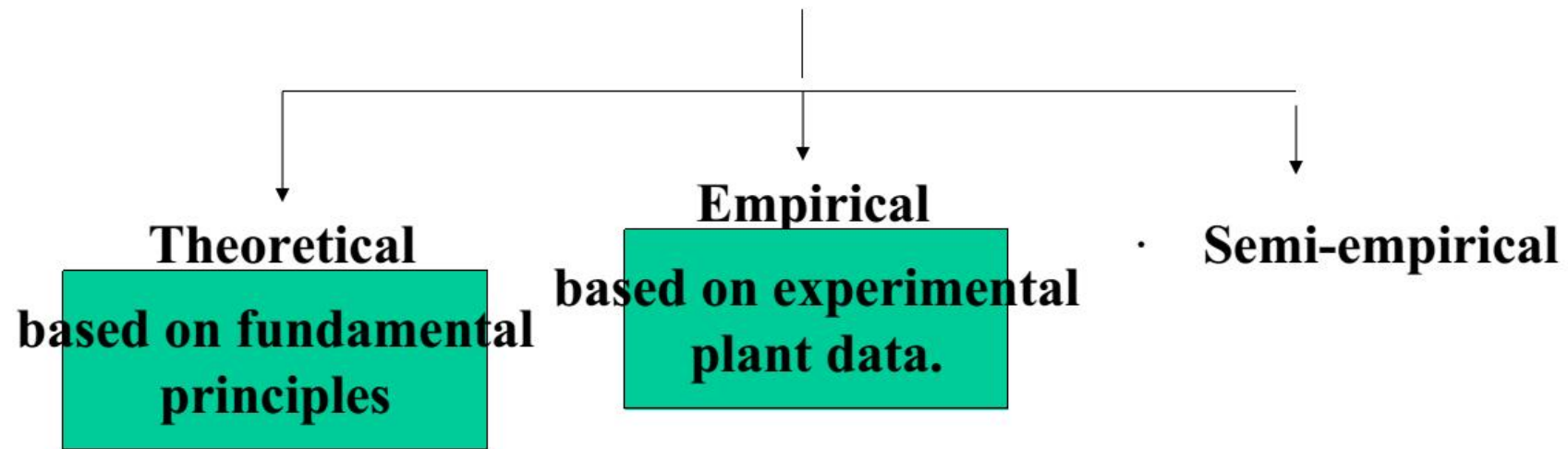
## ❑ Classification based on thermodynamic principles

- i. Isolated system.
- ii. Closed system.
- iii. Open system.

## ❑ Classification based on number of phases

- a. Homogeneous system.
- b. Heterogeneous system.

# Model



**Steady state VS. dynamic**  
**Lumped VS. distributed parameters**  
**Linear Vs Non-linear**  
**Continuous VS discrete**  
**Deterministic VS probabilistic models**



# What does “Steady state and Dynamic” means?

- ❑ **Dynamic:** In all processes of interest, the operating conditions (e.g., temperature, pressure, composition) inside a process unit will be varying over time.
- ❑ **Steady-state:** process variables will not be varying with time

# Why Dynamic Behaviour?

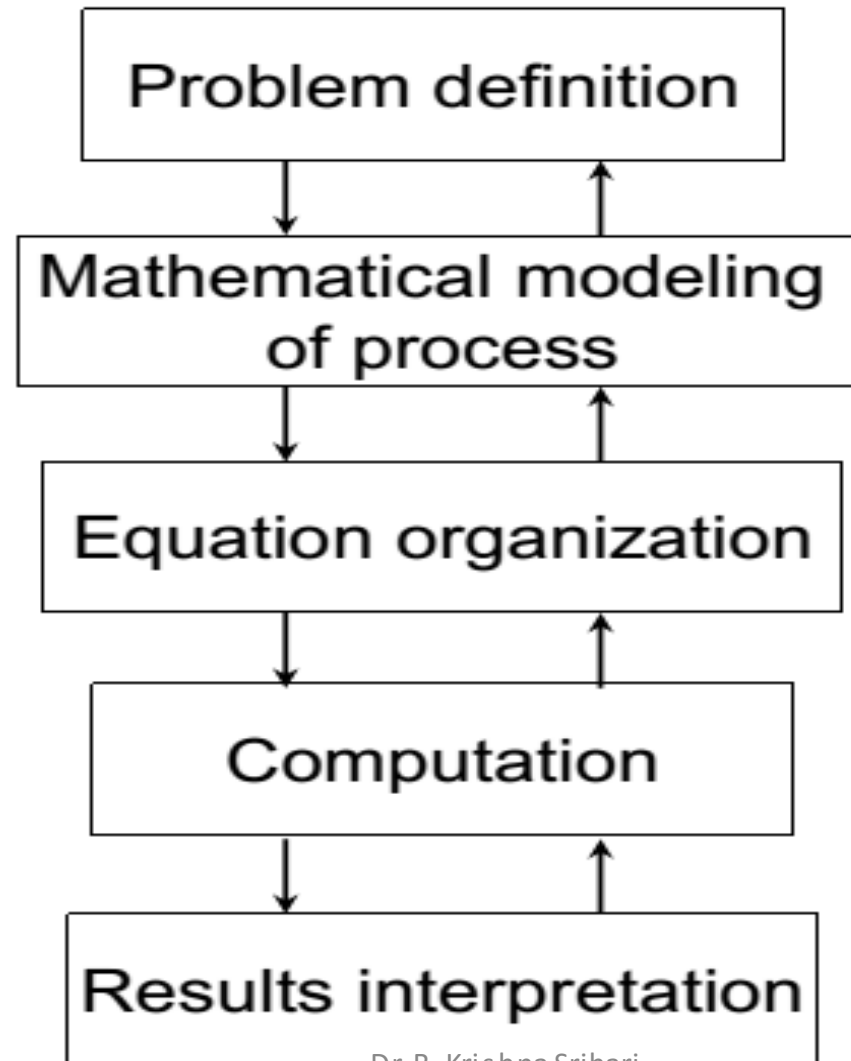
A subject of great importance for the:

1. Study of operability and controllability of continuous processes subject to small disturbances
2. Development of start-up and shut-down procedures
3. Study of switching continuous processes from one steady-state to another
4. Analysis of the safety of processes subject to large disturbances
5. Study of the design and operation procedures for intrinsically dynamic processes (batch/periodic/separation)

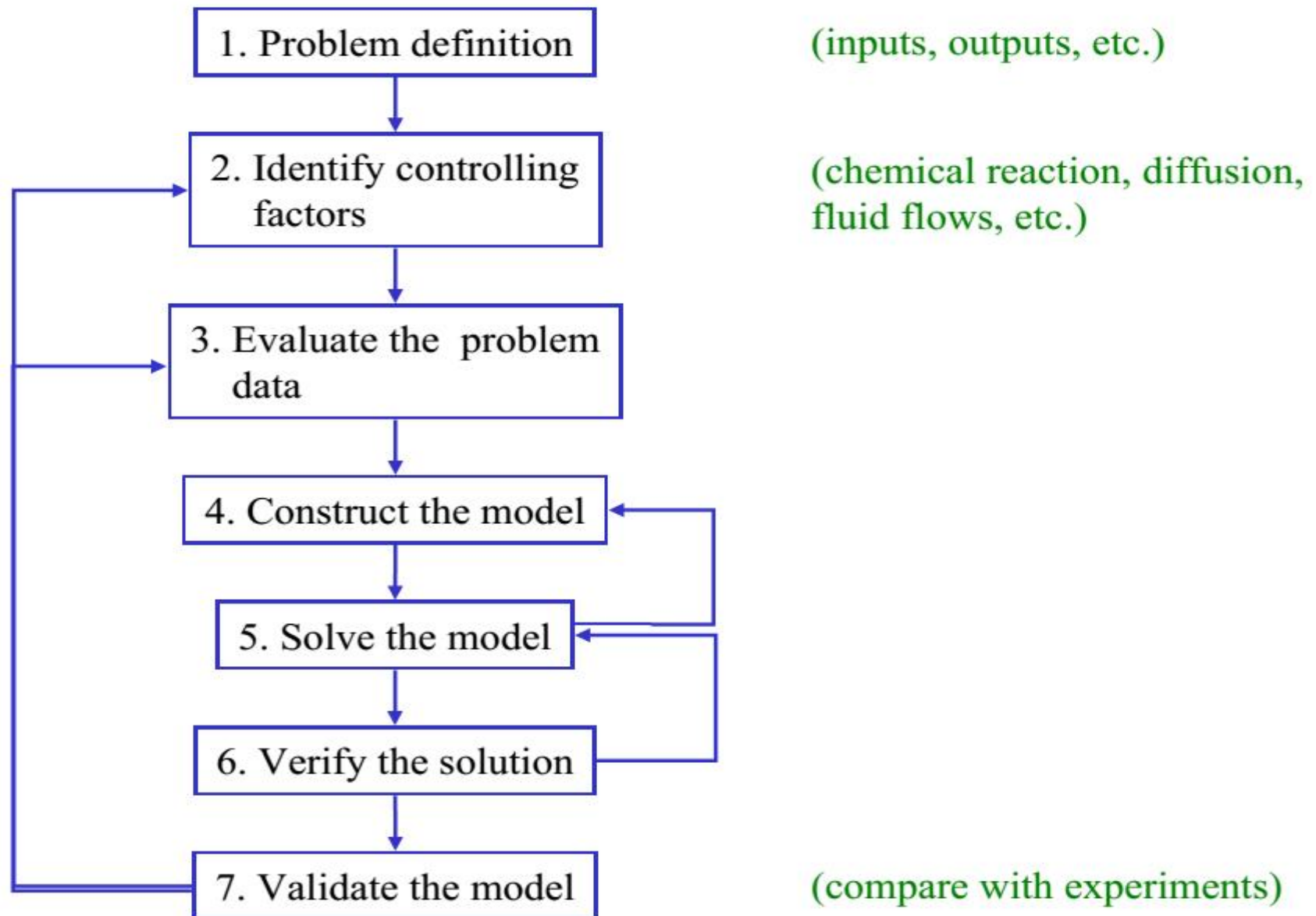
# Impact of simulation on chemical process industry...

- ❑ **Economic:** cheaper to use simulation than to build numerous different-size pilot-plants
- ❑ **Operation:** Easier to develop alternative operating approaches via a mathematical model than by experimental methods
- ❑ **Scale up:** First-principles simulations can predict system performance in new and different operating conditions

# Strategy for simulation of complex chemical processes...



# Systematic Model Building



# Strategy for simulation of complex chemical processes...

□ **A good Problem definition comes from**

- ✓ What I really want to find out?
- ✓ What are the important consequences of the simulation?
- ✓ Why is simulation work required?
- ✓ What data are available?
- ✓ What form of model is required?
- ✓ What are system inputs, outputs, states, ...

# Classification of Mathematical Models

Type of model	Classification
Mechanistic	First-principles
Empirical	Trials/experiments
Stochastic	Probabilistic
Deterministic	Cause-effect
Lumped	Independent of space
Distributed	Dependent on space
Linear	Superposition applies
Nonlinear	Superposition does not apply
Continuous	Over continuous time
Discrete	For discrete values of time

# Ingredients of Process Models

## 1. Assumptions

- Time, spatial characteristics
- Flow conditions

## 2. Model equations and characterizing variables

- Mass, energy, momentum

## 3. Initial conditions

## 4. Boundary conditions

## 5. Parameters



# Ingredients of Process Models

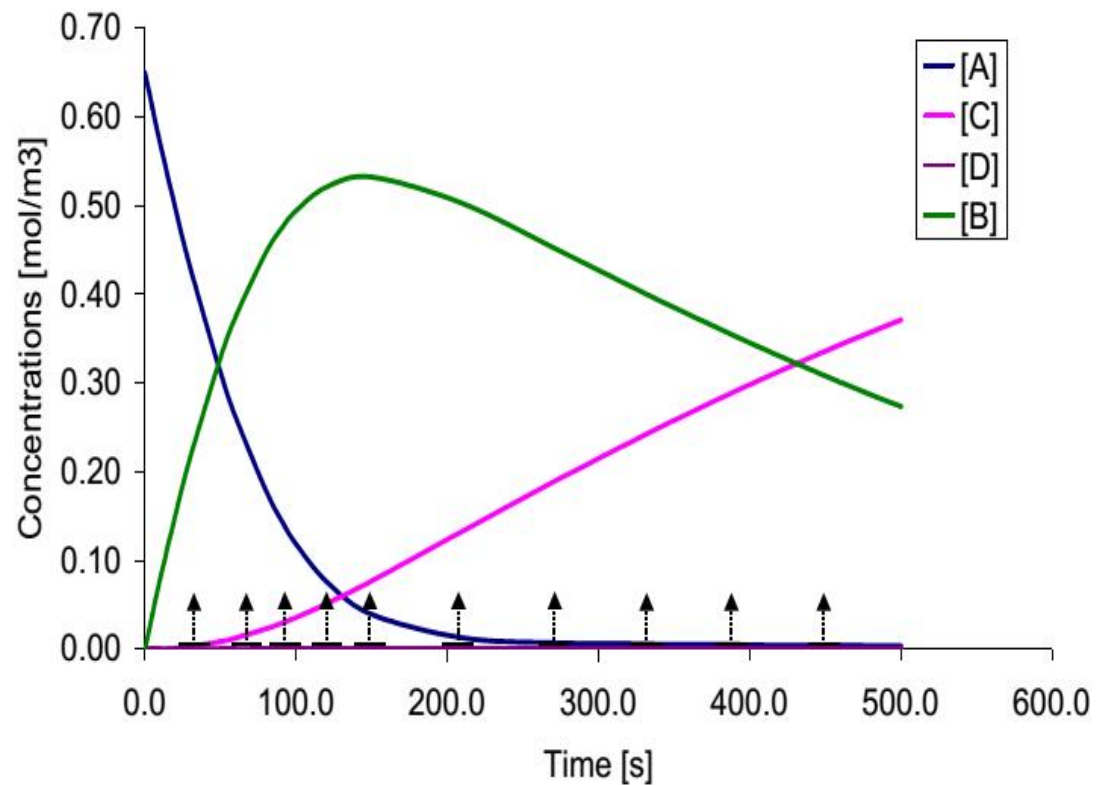
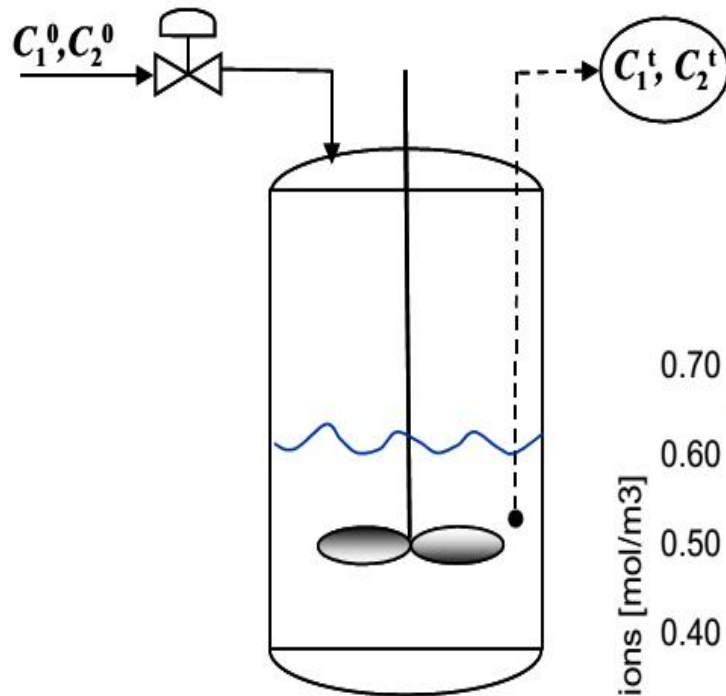
- In mathematics, the field of differential equations, an **initial** value problem (also called the Cauchy problem by some authors) is an ordinary differential equation together with a specified value, called the **initial condition**, of the unknown function at a given point in the domain of the solution.
- In mathematics, in the field of differential equations, a boundary value problem is a differential equation together with a set of additional constraints, called the **boundary conditions**

# Process Classification: Batch vs. Continuous

## ❑ Batch Process:

- ❑ feedstocks for each processing step (i.e., reaction, distillation) are charged into the equipment at the start of processing; products are removed at the end of processing
- ❑ Transfer of material from one item of equipment to the next occurs discontinuously often via intermediate storage tanks
- ❑ Batch processes are intrinsically dynamic conditions within the equipment vary over the duration of the batch

# Batch Process Example: Batch Reactor



# Variations on Batch Operation

## **Semi-batch:**

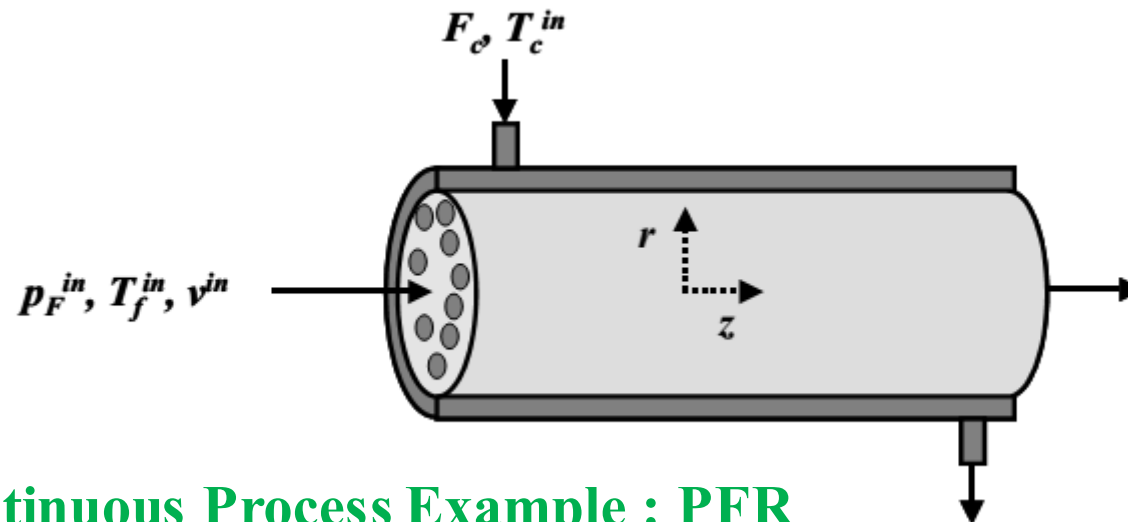
- One or more feedstocks to a batch unit operation to be added during the batch

## **Semi-continuous:**

- Some of the products are removed during the batch

# Continuous Process

- ❑ Involve continuous flows of material from one processing unit to the next
- ❑ Usually designed to operate at steady-state; due to external disturbances, even continuous processes operate dynamically



**Continuous Process Example : PFR**

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# Variation on Continuous OPERATION

## ❑ **Periodic:**

❑ Continuous processes subjected to a periodic (e.g., sinusoidal or square wave) variation of one or more of the material/energy input streams

## ❑ **Industrially Important Examples**

❑ **Periodic adsorption** – periodic conditions (pressure/temperature) regulates preferential adsorption and desorption of different species over different parts of the cycle

❑ **Periodic catalytic reaction** – involves variation of feed composition; under certain conditions the average performance of the reactor is improved

# Lumped vs. Distributed

## ❑ Lumped Operations:

❑ **Perfect mixing**— at any particular time instant, the values of operating conditions are (approximately) the same at all points within the unit

## ❑ Distributed Operations:

❑ **Imperfect mixing** will result in different operating conditions at different points even at the same time → existence of distributions of conditions over spatial domains

# Lumped vs. Distributed : Mathematical Considerations

## ❑ Lumped Operations:

- ❑ Characterized by a single independent variable (time)
- ❑ Their modelling can be effected in terms of ordinary differential equations (ODEs)

## ❑ Distributed Operations:

- ❑ Introduce additional independent variables (e.g., one or more spatial co-ordinates, particle size, molecular weight, etc.)
- ❑ Involves partial differential equations (PDEs) in time



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# Conservation Laws: General Form

- Conservation laws describe the variation of the amount of a “conserved quantity” within the system over time:

$$\left( \begin{array}{c} \text{rate of} \\ \underline{\text{accumulation}} \\ \text{of conserved} \\ \text{quantity} \\ \text{within system} \end{array} \right) = \left( \begin{array}{c} \text{rate of} \\ \text{flow of} \\ \text{conserved} \\ \text{quantity} \\ \underline{\text{into system}} \end{array} \right) - \left( \begin{array}{c} \text{rate of} \\ \text{flow of} \\ \text{conserved} \\ \text{quantity} \\ \underline{\text{from system}} \end{array} \right) + \left( \begin{array}{c} \text{rate of} \\ \underline{\text{generation of}} \\ \text{conserved} \\ \text{quantity} \\ \text{within system} \end{array} \right)$$

# Conservation Laws

Total mass balance:

$$\text{Rate of Accumulation of total mass} = \text{Rate of total mass in} - \text{Rate of total mass out}$$

Species mass balance:

$$\text{Rate of Accumulation of } i = \text{Rate of } i \text{ in} - \text{Rate of } i \text{ out} + \text{Rate of generation of } i$$

Energy balance:

$$\text{Rate of Accumulation of energy} = \text{Rate of energy in} - \text{Rate of energy out} + \text{Rate of generation of energy}$$

Momentum balance:

$$\text{Rate of Accumulation of momentum} = \text{Rate of momentum in} - \text{Rate of momentum out} + \text{Rate of generation of momentum}$$

# Software's for process simulation

- Universal software:
  - Worksheets – Excel, Calc (Open Office)
  - Mathematical software – MathCAD, Matlab
- Specialized software – process simulators. Equipped with:
  - Data base of apparatus models
  - Data base of components and mixtures properties
  - Solver engine
  - User friendly interface

# Software process simulators

- Some actual process simulators:
  1. ASPEN Tech /HYSYS
  2. ChemCAD
  3. PRO/II
  4. ProSim
  5. COMSOL Multiphysics etc.,

# Introduction: Basic Concepts

- A concept is a unit of thought. Any part of experience that we can organize into an idea is a concept. For example, man's concept of cancer is changing all the time as new medical information is gained as a result of experiments.
- Concepts or ideas that are the basis of science and engineering are chemical species, mass, momentum, and energy. A conserved quantity is one which can be transformed. However, transformation does not alter the total amount of the quantity.
- For example, money can be transferred from a checking account to a savings account but the transfer does not affect the total assets.
- For any quantity that is conserved, an inventory rate equation can be written to describe the transformation of the conserved quantity.
- Inventory of the conserved quantity is based on a specified unit of time, which is reflected in the term, rate. In words, this rate equation for any conserved quantity  $\phi$  takes the form

$$\left( \begin{array}{c} \text{Rate of} \\ \text{input of } \varphi \end{array} \right) - \left( \begin{array}{c} \text{Rate of} \\ \text{output of } \varphi \end{array} \right) + \left( \begin{array}{c} \text{Rate of} \\ \text{generation of } \varphi \end{array} \right) = \left( \begin{array}{c} \text{Rate of} \\ \text{accumulation of } \varphi \end{array} \right) \quad (1.1-1)$$

➤ **Basic concepts upon which the technique for solving engineering problems is based are the rate equations for the**

- Conservation of chemical species,
- Conservation of mass,
- Conservation of momentum,
- Conservation of energy.

➤ **Characteristics of the Basic Concepts**

- The basic concepts have certain characteristics that are always taken for granted but seldom stated explicitly. The basic concepts are
  - Independent of the level of application,
  - Independent of the coordinate system to which they are applied,
  - Independent of the substance to which they are applied.

**Table 1.1.** Levels of application of the basic concepts

Level	Theory	Experiment
Microscopic	Equations of Change	Constitutive Equations
Macroscopic	Design Equations	Process Correlations

The basic concepts are applied at both the microscopic and the macroscopic levels as shown in Table 1.1.

At the microscopic level, the basic concepts appear as partial differential equations in three independent space variables and time. Basic concepts at the microscopic level are called the *equations of change*, i.e., conservation of chemical species, mass, momentum, and energy.

Any mathematical description of the response of a material to spatial gradients is called a *constitutive equation*. Just as the reaction of different people to the same joke may vary, the response of materials to the variable condition in a process differs. Constitutive equations are postulated and cannot be derived from the fundamental principles<sup>1</sup>. The coefficients appearing in the constitutive equations are obtained from experiments.

Integration of the equations of change over an arbitrary engineering volume exchanging mass and energy with the surroundings gives the basic concepts at the macroscopic level. The resulting equations appear as ordinary differential equations, with time as the only independent variable. The basic concepts at this level are called the *design equations* or *macroscopic balances*. For example, when the microscopic level mechanical energy balance is integrated over an arbitrary engineering volume, the result is the macroscopic level engineering Bernoulli equation.



Constitutive equations, when combined with the equations of change, may or may not comprise a determinate mathematical system. For a determinate mathematical system, i.e., the number of unknowns is equal to the number of independent equations, the solutions of the equations of change together with the constitutive equations result in the velocity, temperature, pressure, and concentration profiles within the system of interest. These profiles are called *theoretical (or analytical) solutions*. A theoretical solution enables one to design and operate a process without resorting to experiments or scale-up. Unfortunately, the number of such theoretical solutions is small relative to the number of engineering problems that must be solved.

If the required number of constitutive equations is not available, i.e., the number of unknowns is greater than the number of independent equations, then the mathematical description at the microscopic level is indeterminate. In this case, the design procedure appeals to an experimental information called *process correlation* to replace the theoretical solution. All process correlations are limited to a specific geometry, equipment configuration, boundary conditions, and substance.

# Definitions

## 1.2.1 Steady-State

The term steady-state means that at a particular location in space the dependent variable does not change as a function of time. If the dependent variable is  $\varphi$ , then

$$\left(\frac{\partial\varphi}{\partial t}\right)_{x,y,z} = 0 \quad (1.2-2)$$

The partial derivative notation indicates that the dependent variable is a function of more than one independent variable. In this particular case, the independent variables are  $(x, y, z)$  and  $t$ . The specified location in space is indicated by the subscripts  $(x, y, z)$ , and Eq. (1.2-2) implies that  $\varphi$  is not a function of time,  $t$ . When an ordinary derivative is used, i.e.,  $d\varphi/dt = 0$ , then this implies that  $\varphi$  is a constant. It is important to distinguish between partial and ordinary derivatives because the conclusions are very different.

**Example 1.2** A cylindrical tank is initially half full with water. The water is fed into the tank from the top and it leaves the tank from the bottom. The inlet and outlet volumetric flow rates are different from each other. The differential equation describing the time rate of change of water height is given by

$$\frac{dh}{dt} = 6 - 8\sqrt{h}$$

where  $h$  is the height of water in meters. Calculate the height of water in the tank under steady conditions.

**Solution**

Under steady conditions  $dh/dt$  must be zero. Then

$$0 = 6 - 8\sqrt{h}$$

or,

$$h = 0.56 \text{ m}$$

### 1.2.2 Uniform

The term *uniform* means that at a particular instant in time, the dependent variable is not a function of position. This requires that all three of the partial derivatives with respect to position be zero, i.e.,

$$\left(\frac{\partial\varphi}{\partial x}\right)_{y,z,t} = \left(\frac{\partial\varphi}{\partial y}\right)_{x,z,t} = \left(\frac{\partial\varphi}{\partial z}\right)_{x,y,t} = 0 \quad (1.2-3)$$

The variation of a physical quantity with respect to position is called *gradient*. Therefore, the gradient of a quantity must be zero for a uniform condition to exist with respect to that quantity.

### 1.2.3 Equilibrium

A system is in *equilibrium* if both steady-state and uniform conditions are met simultaneously. An equilibrium system does not exhibit any variation with respect to position or time. The state of an equilibrium system is specified completely by the non-Euclidean coordinates<sup>2</sup> ( $P, V, T$ ). The response of a material under equilibrium conditions is called *property correlation*. The ideal gas law is an example of a thermodynamic property correlation that is called an *equation of state*.

### 1.2.4 Flux

The flux of a certain quantity is defined by

$$\text{Flux} = \frac{\text{Flow of a quantity/Time}}{\text{Area}} = \frac{\text{Flow rate}}{\text{Area}} \quad (1.2-4)$$

where area is normal to the direction of flow. The units of momentum, energy, mass, and molar fluxes are Pa (N/m<sup>2</sup>, or kg/m·s<sup>2</sup>), W/m<sup>2</sup> [(J/m<sup>2</sup>·s)], kg/m<sup>2</sup>·s, and kmol/m<sup>2</sup>·s, respectively.

### 1.3 MATHEMATICAL FORMULATION OF THE BASIC CONCEPTS

In order to obtain the mathematical description of a process, the general inventory rate equation given by Eq. (1.1-1) should be translated into mathematical terms.

#### 1.3.1 Inlet and Outlet Terms

A quantity may enter or leave the system by two means: (i) by inlet and/or outlet streams, (ii) by exchange of a particular quantity between the system and its surroundings through the boundaries of the system. In either case, the rate of input and/or output of a quantity is expressed by using the flux of that particular quantity. The flux of a quantity may be constant or dependent on position. Thus, the rate of a quantity can be determined as

$$\text{Inlet/Outlet rate} = \begin{cases} (\text{Flux})(\text{Area}) & \text{if flux is constant} \\ \iint_A \text{Flux } dA & \text{if flux is position dependent} \end{cases} \quad (1.3-1)$$

where  $A$  is the area perpendicular to the direction of the flux. The differential areas in cylindrical and spherical coordinate systems are given in Section A.1 in Appendix A.

### 1.3.2 Rate of Generation Term

The generation rate per unit volume is denoted by  $\mathfrak{R}$  and it may be constant or dependent on position. Thus, the generation rate is expressed as

$$\text{Generation rate} = \begin{cases} (\mathfrak{R})(\text{Volume}) & \text{if } \mathfrak{R} \text{ is constant} \\ \iiint_V \mathfrak{R} dV & \text{if } \mathfrak{R} \text{ is position dependent} \end{cases} \quad (1.3-2)$$

where  $V$  is the volume of the system in question. It is also possible to have the depletion of a quantity. In that case, the plus sign in front of the generation term must be replaced by the minus sign, i.e.,

$$\text{Depletion rate} = - \text{Generation rate} \quad (1.3-3)$$

### 1.3.3 Rate of Accumulation Term

The rate of accumulation of any quantity  $\varphi$  is the time rate of change of that particular quantity within the volume of the system. Let  $\rho$  be the mass density and  $\hat{\varphi}$  be the quantity per unit mass. Thus,

$$\text{Total quantity of } \varphi = \iiint_V \rho \hat{\varphi} dV \quad (1.3-4)$$

and the rate of accumulation is given by

$$\text{Accumulation rate} = \frac{d}{dt} \left( \iiint_V \rho \hat{\varphi} dV \right) \quad (1.3-5)$$

If  $\hat{\varphi}$  is independent of position, then Eq. (1.3-5) simplifies to

$$\text{Accumulation rate} = \frac{d}{dt} (m \hat{\varphi}) \quad (1.3-6)$$

where  $m$  is the total mass within the system.

The accumulation rate may be positive or negative depending on whether the quantity is increasing or decreasing with time within the volume of the system.

## 1.4 SIMPLIFICATION OF THE RATE EQUATION

In this section, the general rate equation given by Eq. (1.1-1) will be simplified for two special cases: (i) steady-state transport without generation, (ii) steady-state transport with generation.

### 1.4.1 Steady-State Transport Without Generation

For this case Eq. (1.1-1) reduces to

$$\text{Rate of input of } \varphi = \text{Rate of output of } \varphi \quad (1.4-1)$$

Equation (1.4-1) can also be expressed in terms of flux as

$$\iint_{A_{in}} (\text{Inlet flux of } \varphi) dA = \iint_{A_{out}} (\text{Outlet flux of } \varphi) dA \quad (1.4-2)$$

For constant inlet and outlet fluxes Eq. (1.4-2) reduces to

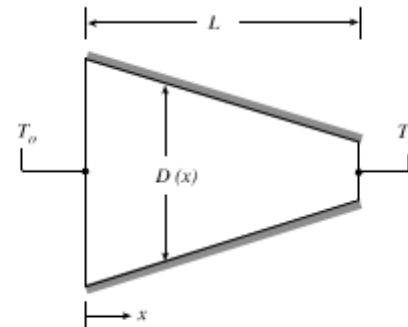
$$\left( \begin{array}{c} \text{Inlet flux} \\ \text{of } \varphi \end{array} \right) \left( \begin{array}{c} \text{Inlet} \\ \text{area} \end{array} \right) = \left( \begin{array}{c} \text{Outlet flux} \\ \text{of } \varphi \end{array} \right) \left( \begin{array}{c} \text{Outlet} \\ \text{area} \end{array} \right) \quad (1.4-3)$$

If the inlet and outlet areas are equal, then Eq. (1.4-3) becomes

$$\text{Inlet flux of } \varphi = \text{Outlet flux of } \varphi \quad (1.4-4)$$

It is important to note that Eq. (1.4-4) is valid as long as the areas perpendicular to the direction of flow at the inlet and outlet of the system are equal to each other. The variation of the area in between does not affect this conclusion. Equation (1.4-4) obviously is not valid for the transfer processes taking place in the radial direction in cylindrical and spherical coordinate systems. In this case either Eq. (1.4-2) or Eq. (1.4-3) should be used.





**Figure 1.2.** Heat transfer through a solid circular cone.

**Example 1.5** Consider a solid cone of circular cross-section whose lateral surface is well insulated as shown in Figure 1.2. The diameters at  $x = 0$  and  $x = L$  are 25 cm and 5 cm, respectively. If the heat flux at  $x = 0$  is  $45 \text{ W/m}^2$  under steady conditions, determine the heat transfer rate and the value of the heat flux at  $x = L$ .

**Solution**

For steady-state conditions without generation, the heat transfer rate is constant and can be determined from Eq. (1.3-1) as

$$\text{Heat transfer rate} = (\text{Heat flux})_{x=0}(\text{Area})_{x=0}$$

Since the cross-sectional area of the cone is  $\pi D^2/4$ , then

$$\text{Heat transfer rate} = (45) \left[ \frac{\pi (0.25)^2}{4} \right] = 2.21 \text{ W}$$

The value of the heat transfer rate is also 2.21 W at  $x = L$ . However, the heat flux does depend on position and its value at  $x = L$  is

$$(\text{Heat flux})_{x=L} = \frac{2.21}{[\pi (0.05)^2/4]} = 1126 \text{ W/m}^2$$

**Comment:** Heat flux values are different from each other even though the heat flow rate is constant. Therefore, it is important to specify the area upon which a given heat flux is based when the area changes as a function of position.

### 1.4.2 Steady-State Transport with Generation

For this case Eq. (1.1-1) reduces to

$$\left( \begin{array}{c} \text{Rate of} \\ \text{input of } \varphi \end{array} \right) + \left( \begin{array}{c} \text{Rate of} \\ \text{generation of } \varphi \end{array} \right) = \left( \begin{array}{c} \text{Rate of} \\ \text{output of } \varphi \end{array} \right) \quad (1.4-5)$$

Equation (1.4-5) can also be written in the form

$$\iint_{A_{in}} (\text{Inlet flux of } \varphi) dA + \iiint_{V_{sys}} \mathfrak{R} dV = \iint_{A_{out}} (\text{Outlet flux of } \varphi) dA \quad (1.4-6)$$

where  $\mathfrak{R}$  is the generation rate per unit volume. If the inlet and outlet fluxes together with the generation rate are constant, then Eq. (1.4-6) reduces to

$$\left( \begin{array}{c} \text{Inlet flux} \\ \text{of } \varphi \end{array} \right) \left( \begin{array}{c} \text{Inlet} \\ \text{area} \end{array} \right) + \mathfrak{R} \left( \begin{array}{c} \text{System} \\ \text{volume} \end{array} \right) = \left( \begin{array}{c} \text{Outlet flux} \\ \text{of } \varphi \end{array} \right) \left( \begin{array}{c} \text{Outlet} \\ \text{area} \end{array} \right) \quad (1.4-7)$$

**Example 1.6** An exothermic chemical reaction takes place in a 20 cm thick slab and the energy generation rate per unit volume is  $1 \times 10^6 \text{ W/m}^3$ . The steady-state heat transfer rate into the slab at the left-hand side, i.e., at  $x = 0$ , is 280 W. Calculate the heat transfer rate to the surroundings from the right-hand side of the slab, i.e., at  $x = L$ . The surface area of each face is  $40 \text{ cm}^2$ .

### Solution

At steady-state, there is no accumulation of energy and the use of Eq. (1.4-5) gives

$$\begin{aligned}(\text{Heat transfer rate})_{x=L} &= (\text{Heat transfer rate})_{x=0} + \dot{q} (\text{Volume}) \\ &= 280 + (1 \times 10^6)(40 \times 10^{-4})(20 \times 10^{-2}) = 1080 \text{ W}\end{aligned}$$

The values of the heat fluxes at  $x = 0$  and  $x = L$  are

$$\begin{aligned}(\text{Heat flux})_{x=0} &= \frac{280}{40 \times 10^{-4}} = 70 \times 10^3 \text{ W/m}^2 \\ (\text{Heat flux})_{x=L} &= \frac{1080}{40 \times 10^{-4}} = 270 \times 10^3 \text{ W/m}^2\end{aligned}$$

**Comment:** Even though the steady-state conditions prevail, neither the heat transfer rate nor the heat flux are constant. This is due to the generation of energy within the slab.

## PROBLEMS

1.1 One of your friends writes down the inventory rate equation for money as

$$\left( \begin{array}{c} \text{Change in amount} \\ \text{of dollars} \end{array} \right) = (\text{Interest}) - \left( \begin{array}{c} \text{Service} \\ \text{charge} \end{array} \right) + \left( \begin{array}{c} \text{Dollars} \\ \text{deposited} \end{array} \right) - \left( \begin{array}{c} \text{Checks} \\ \text{written} \end{array} \right)$$

Identify the terms in the above equation.

### Answer

Rate of Accumulation = (Rate of generation) - (Rate of disappearance) + (Rate of Input) - (Rate of Output)

1.2 Determine whether steady- or unsteady-state conditions prevail for the following cases:

- a) The height of water in a dam during heavy rain,
- b) The weight of an athlete during a marathon,
- c) The temperature of an ice cube as it melts.

### Answer

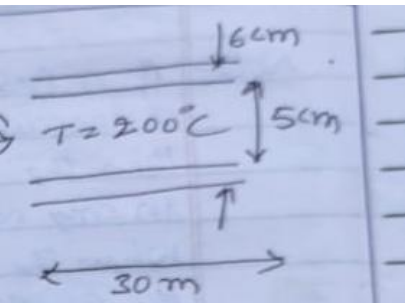
(a) Unsteady state    (b) Steady Sate    (c) Steady state

1.4 Steam at a temperature of  $200^{\circ}\text{C}$  flows through a pipe of 5 cm inside diameter and 6 cm outside diameter. The length of the pipe is 30 m. If the steady rate of heat loss per unit length of the pipe is  $2\text{ W/m}$ , calculate the heat fluxes at the inner and outer surfaces of the pipe.

(Answer:  $12.7\text{ W/m}^2$  and  $10.6\text{ W/m}^2$ )

### Answers

PMS



1.4 Ans

Given,

Inside dia. of Pipe ( $d_i$ ) =  $5\text{ cm} = 0.05\text{ m}$   
 outside dia. of Pipe ( $d_o$ ) =  $6\text{ cm} = 0.06\text{ m}$   
 Length of the Pipe ( $L$ ) =  $30\text{ m}$

Area based on inside diameter ( $A_i$ ) =  $\pi d_i L = \pi \times 0.05 \times 30$   
 $= 4.712\text{ m}^2$

Area based on outside diameter ( $A_o$ ) =  $\pi d_o L$   
 $= \pi \times 0.06 \times 30$   
 $= 5.655\text{ m}^2$

Rate of heat loss per unit length of pipe  
 $= 2\text{ W/m}$

Total rate of heat loss from the total surface of the pipe ( $Q$ ) =  $\frac{\text{Rate of heat loss per unit length}}{\text{Length}} \times \text{Length of the pipe}$

$$Q = 2 \frac{\text{W}}{\text{m}} \times 30 \text{ m}$$

$$Q = 60 \text{ W}$$

DATE: / / 20

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We know, Flux =  $\frac{\text{Rate}}{\text{Area}}$

① Heat flux at inner surface of the pipe

$$= \frac{Q}{A_i} = \frac{60 \text{ W}}{4.172 \text{ m}^2}$$

$$= 12.73 \text{ W/m}^2$$

② Heat flux at outer surface of the pipe

$$= \frac{Q}{A_o} = \frac{60 \text{ W}}{5.655 \text{ m}^2}$$

$$= 10.61 \text{ W/m}^2$$

1.5 Dust evolves at a rate of 0.3 kg/h in a foundry of dimensions 20 m × 8 m × 4 m. According to ILO (International Labor Organization) standards, the dust concentration should not exceed 20 mg/m<sup>3</sup> to protect workers' health. Determine the volumetric flow rate of ventilating air to meet the standards of ILO.

(Answer: 15,000 m<sup>3</sup>/h)

Given,  
(1.5) Ans) Rate of dust evolves = Rate of generation  
of dust = 0.3 kg/h,  
Dimensions = 20 m × 8 m × 4 m  
(Volume of Foundry) ↑  
The dust conc<sup>n</sup> shd not exceed =  $C_p$  (or)  $C_0$   
 $= \frac{20 \text{ mg}}{\text{m}^3}$   
 $= 20 \times 10^{-6} \frac{\text{kg}}{\text{m}^3}$

on basis of dust, mass balance of dust,

$$\left( \begin{array}{l} \text{Rate of I/P} \\ \text{of dust} \end{array} \right) - \left( \begin{array}{l} \text{Rate of o/p} \\ \text{of dust} \end{array} \right) + \left( \begin{array}{l} \text{Rate of generation} \\ \text{of dust} \end{array} \right) \\ = \left( \begin{array}{l} \text{Rate of accumulation} \\ \text{of dust} \end{array} \right)$$

Assume process is steady state, so, no accumulation term and initial concn of dust is equal to zero  $= c_i = 0$

so,  $c_i Q_i = 0$

$$c_i Q_i - c_o Q_o + RV = 0$$

$$(-20 \times 10^{-6} \times Q_o) + 0.3 \text{ kg/h} = 0$$

$$Q_o = \frac{0.3}{20 \times 10^{-6}} = \boxed{15,000 \text{ m}^3/\text{h}}$$

↓  
volumetric flow rate of ventilating air to meet the standards



## 2

---

# MOLECULAR AND CONVECTIVE TRANSPORT

The total flux of any quantity is the sum of the molecular and convective fluxes. The fluxes arising from potential gradients or driving forces are called *molecular fluxes*. Molecular fluxes are expressed in the form of *constitutive* (or *phenomenological*) *equations* for momentum, energy, and mass transport. Momentum, energy, and mass can also be transported by bulk fluid motion or bulk flow, and the resulting flux is called *convective flux*. This chapter deals with the formulation of molecular and convective fluxes in momentum, energy, and mass transport.

### 2.1 MOLECULAR TRANSPORT

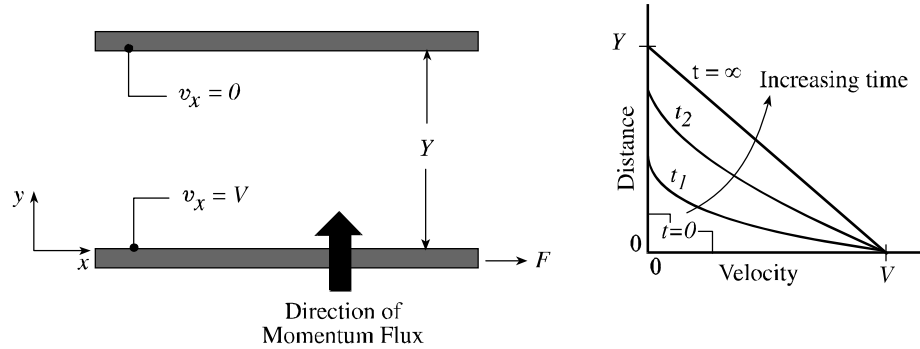
Substances may behave differently when subjected to the same gradients. *Constitutive equations* identify the characteristics of a particular substance. For example, if the gradient is momentum, then the viscosity is defined by the constitutive equation called *Newton's law of viscosity*. If the gradient is energy, then the thermal conductivity is defined by *Fourier's law of heat conduction*. If the gradient is concentration, then the diffusion coefficient is defined by *Fick's first law of diffusion*. Viscosity, thermal conductivity, and diffusion coefficient are called *transport properties*.

#### 2.1.1 Newton's Law of Viscosity

Consider a fluid contained between two large parallel plates of area  $A$ , separated by a very small distance  $Y$ . The system is initially at rest but at time  $t = 0$  the lower plate is set in motion in the  $x$ -direction at a constant velocity  $V$  by applying a force  $F$  in the  $x$ -direction while the upper plate is kept stationary. The resulting velocity profiles are shown in Figure 2.1 for various times. At  $t = 0$ , the velocity is zero everywhere except at the lower plate, which has a velocity  $V$ . Then the velocity distribution starts to develop as a function of time. Finally, at steady-state, a linear velocity distribution is obtained.

Experimental results show that the force required to maintain the motion of the lower plate per unit area (or momentum flux) is proportional to the velocity gradient, i.e.,

$$\underbrace{\frac{F}{A}}_{\text{Momentum flux}} = \underbrace{\mu}_{\text{Transport property}} \underbrace{\frac{V}{Y}}_{\text{Velocity gradient}} \quad (2.1-1)$$



**Figure 2.1.** Velocity profile development in flow between parallel plates.

and the proportionality constant,  $\mu$ , is the *viscosity*. Equation (2.1-1) is a macroscopic equation. The microscopic form of this equation is given by

$$\tau_{yx} = -\mu \frac{dv_x}{dy} = -\mu \dot{\gamma}_{yx} \quad (2.1-2)$$

which is known as *Newton's law of viscosity* and any fluid obeying Eq. (2.1-2) is called a *Newtonian fluid*. The term  $\dot{\gamma}_{yx}$  is called *rate of strain*<sup>1</sup> or *rate of deformation* or *shear rate*. The term  $\tau_{yx}$  is called *shear stress*. It contains two subscripts:  $x$  represents the direction of force, i.e.,  $F_x$ , and  $y$  represents the direction of the normal to the surface, i.e.,  $A_y$ , on which the force is acting. Therefore,  $\tau_{yx}$  is simply the force per unit area, i.e.,  $F_x/A_y$ . It is also possible to interpret  $\tau_{yx}$  as the flux of  $x$ -momentum in the  $y$ -direction.

Since the velocity gradient is negative, i.e.,  $v_x$  decreases with increasing  $y$ , a negative sign is introduced on the right-hand side of Eq. (2.1-2) so that the stress in tension is positive.

In SI units, shear stress is expressed in  $\text{N/m}^2$  (Pa) and velocity gradient in  $(\text{m/s})/\text{m}$ . Thus, the examination of Eq. (2.1-1) indicates that the units of viscosity in SI units are

$$\mu = \frac{\text{N/m}^2}{(\text{m/s})/\text{m}} = \text{Pa}\cdot\text{s} = \frac{\text{N}\cdot\text{s}}{\text{m}^2} = \frac{(\text{kg}\cdot\text{m/s}^2)\cdot\text{s}}{\text{m}^2} = \frac{\text{kg}}{\text{m}\cdot\text{s}}$$

Most viscosity data in the cgs system are usually reported in  $\text{g}/(\text{cm}\cdot\text{s})$ , known as a poise (P), or in centipoise ( $1 \text{ cP} = 0.01 \text{ P}$ ), where

$$1 \text{ Pa}\cdot\text{s} = 10 \text{ P} = 10^3 \text{ cP}$$

Viscosity varies with temperature. While liquid viscosity decreases with increasing temperature, gas viscosity increases with increasing temperature. Concentration also affects viscosity for solutions or suspensions. Viscosity values of various substances are given in Table D.1 in Appendix D.

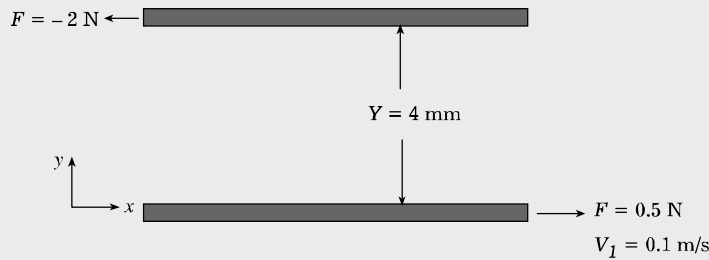
**Example 2.1** A Newtonian fluid with a viscosity of 10 cP is placed between two large parallel plates. The distance between the plates is 4 mm. The lower plate is pulled in the positive  $x$ -direction with a force of 0.5 N, while the upper plate is pulled in the negative

<sup>1</sup>Strain is defined as deformation per unit length. For example, if a spring of original length  $L_0$  is stretched to a length  $L$ , then the strain is  $(L - L_0)/L_0$ .

$x$ -direction with a force of 2 N. Each plate has an area of  $2.5 \text{ m}^2$ . If the velocity of the lower plate is  $0.1 \text{ m/s}$ , calculate:

- The steady-state momentum flux,
- The velocity of the upper plate.

### Solution



- The momentum flux (or force per unit area) is

$$\tau_{yx} = \frac{F}{A} = \frac{0.5 + 2}{2.5} = 1 \text{ Pa}$$

- Let  $V_2$  be the velocity of the upper plate. From Eq. (2.1-2)

$$\tau_{yx} \int_0^Y dy = -\mu \int_{V_1}^{V_2} dv_x \quad \Rightarrow \quad V_2 = V_1 - \frac{\tau_{yx} Y}{\mu} \quad (1)$$

Substitution of the values into Eq. (1) gives

$$V_2 = 0.1 - \frac{(1)(4 \times 10^{-3})}{10 \times 10^{-3}} = -0.3 \text{ m/s} \quad (2)$$

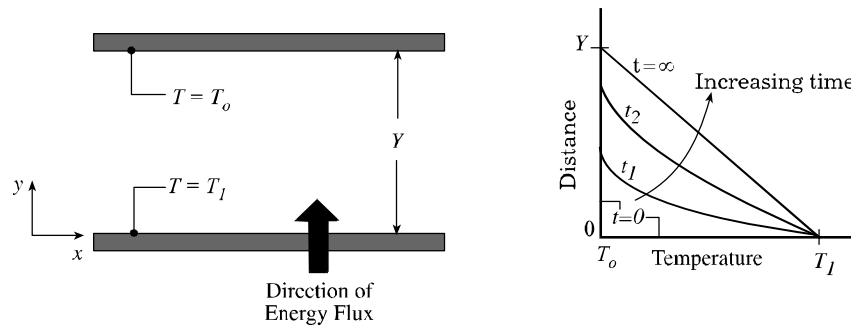
The minus sign indicates that the upper plate moves in the negative  $x$ -direction. Note that the velocity gradient is  $dv_x/dy = -100 \text{ s}^{-1}$ .

### 2.1.2 Fourier's Law of Heat Conduction

Consider a slab of solid material of area  $A$  between two large parallel plates of a distance  $Y$  apart. Initially the solid material is at temperature  $T_o$  throughout. Then the lower plate is suddenly brought to a slightly higher temperature,  $T_1$ , and maintained at that temperature. The second law of thermodynamics states that heat flows spontaneously from the higher temperature  $T_1$  to the lower temperature  $T_o$ . As time proceeds, the temperature profile in the slab changes, and ultimately a linear steady-state temperature is attained as shown in Figure 2.3.

Experimental measurements made at steady-state indicate that the rate of heat flow per unit area is proportional to the temperature gradient, i.e.,

$$\underbrace{\frac{\dot{Q}}{A}}_{\text{Energy flux}} = \underbrace{k}_{\text{Transport property}} \underbrace{\frac{T_1 - T_o}{Y}}_{\text{Temperature gradient}} \quad (2.1-3)$$



**Figure 2.3.** Temperature profile development in a solid slab between two plates.

The proportionality constant,  $k$ , between the energy flux and the temperature gradient is called *thermal conductivity*. In SI units,  $\dot{Q}$  is in W(J/s),  $A$  in  $m^2$ ,  $dT/dx$  in K/m, and  $k$  in  $W/m \cdot K$ . The thermal conductivity of a material is, in general, a function of temperature. However, in many engineering applications the variation is sufficiently small to be neglected. Thermal conductivity values for various substances are given in Table D.2 in Appendix D.

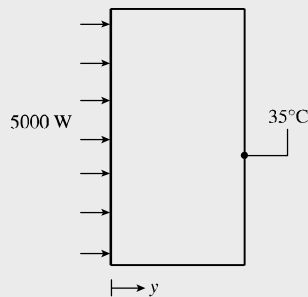
The microscopic form of Eq. (2.1-3) is known as *Fourier's law of heat conduction* and is given by

$$q_y = -k \frac{dT}{dy} \quad (2.1-4)$$

in which the subscript  $y$  indicates the direction of the energy flux. The negative sign in Eq. (2.1-4) indicates that heat flows in the direction of decreasing temperature.

**Example 2.2** One side of a copper slab receives a net heat input at a rate of 5000 W due to radiation. The other face is held at a temperature of 35 °C. If steady-state conditions prevail, calculate the surface temperature of the side receiving radiant energy. The surface area of each face is 0.05  $m^2$ , and the slab thickness is 4 cm.

### Solution



### Physical Properties

For copper:  $k = 398 \text{ W/m} \cdot \text{K}$

**Analysis**

System: Copper slab

Under steady conditions with no internal generation, the conservation statement for energy reduces to

$$\text{Rate of energy in} = \text{Rate of energy out} = 5000 \text{ W}$$

Since the slab area across which heat transfer takes place is constant, the heat flux through the slab is also constant, and is given by

$$q_y = \frac{5000}{0.05} = 100,000 \text{ W/m}^2$$

Therefore, the use of Fourier's law of heat conduction, Eq. (2.1-4), gives

$$100,000 \int_0^{0.04} dy = -398 \int_{T_o}^{35} dT \Rightarrow T_o = 45.1^\circ\text{C}$$

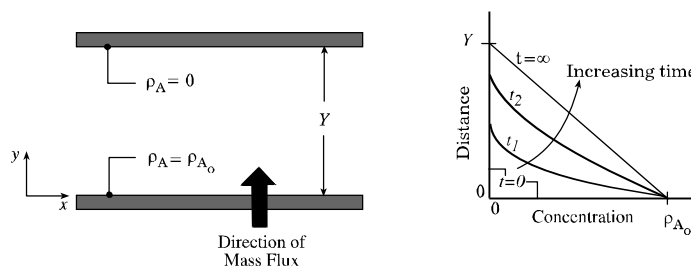
**2.1.3 Fick's First Law of Diffusion**

Consider two large parallel plates of area  $A$ . The lower one is coated with a material,  $\mathcal{A}$ , which has a very low solubility in the stagnant fluid  $\mathcal{B}$  filling the space between the plates. Suppose that the saturation concentration of  $\mathcal{A}$  is  $\rho_{A_o}$  and  $\mathcal{A}$  undergoes a rapid chemical reaction at the surface of the upper plate and its concentration is zero at that surface. At  $t = 0$  the lower plate is exposed to  $\mathcal{B}$  and, as time proceeds, the concentration profile develops as shown in Figure 2.4. Since the solubility of  $\mathcal{A}$  is low, an almost linear distribution is reached under steady conditions.

Experimental measurements indicate that the mass flux of  $\mathcal{A}$  is proportional to the concentration gradient, i.e.,

$$\underbrace{\frac{\dot{m}_A}{A}}_{\text{Mass flux of } \mathcal{A}} = \underbrace{\mathcal{D}_{AB}}_{\text{Transport property}} \underbrace{\frac{\rho_{A_o}}{Y}}_{\text{Concentration gradient}} \quad (2.1-5)$$

where the proportionality constant,  $\mathcal{D}_{AB}$ , is called the *binary molecular mass diffusivity* (or *diffusion coefficient*) of species  $\mathcal{A}$  through  $\mathcal{B}$ . The microscopic form of Eq. (2.1-5) is known



**Figure 2.4.** Concentration profile development between parallel plates.

as Fick's first law of diffusion and is given by

$$j_{A_y} = -\mathcal{D}_{AB}\rho \frac{d\omega_A}{dy} \quad (2.1-6)$$

where  $j_{A_y}$  and  $\omega_A$  represent the molecular mass flux of species  $\mathcal{A}$  in the  $y$ -direction and mass fraction of species  $\mathcal{A}$ , respectively. If the total density,  $\rho$ , is constant, then the term  $\rho(d\omega_A/dy)$  can be replaced by  $d\rho_A/dy$  and Eq. (2.1-6) becomes

$$j_{A_y} = -\mathcal{D}_{AB} \frac{d\rho_A}{dy} \quad \rho = \text{constant} \quad (2.1-7)$$

To measure  $\mathcal{D}_{AB}$  experimentally, it is necessary to design an experiment (like the one given above) in which the convective mass flux is almost zero.

In mass transfer calculations, it is sometimes more convenient to express concentrations in molar units rather than in mass units. In terms of molar concentration, Fick's first law of diffusion is written as

$$J_{A_y}^* = -\mathcal{D}_{AB}c \frac{dx_A}{dy} \quad (2.1-8)$$

where  $J_{A_y}^*$  and  $x_A$  represent the molecular molar flux of species  $\mathcal{A}$  in the  $y$ -direction and the mole fraction of species  $\mathcal{A}$ , respectively. If the total molar concentration,  $c$ , is constant, then the term  $c(dx_A/dy)$  can be replaced by  $dc_A/dy$ , and Eq. (2.1-8) becomes

$$J_{A_y}^* = -\mathcal{D}_{AB} \frac{dc_A}{dy} \quad c = \text{constant} \quad (2.1-9)$$

The diffusion coefficient has the dimensions of  $\text{m}^2/\text{s}$  in SI units. Typical values of  $\mathcal{D}_{AB}$  are given in Appendix D. Examination of these values indicates that the diffusion coefficient of gases has an order of magnitude of  $10^{-5} \text{ m}^2/\text{s}$  under atmospheric conditions. Assuming ideal gas behavior, the pressure and temperature dependence of the diffusion coefficient of gases may be estimated from the relation

$$\mathcal{D}_{AB} \propto \frac{T^{3/2}}{P} \quad (2.1-10)$$

Diffusion coefficients for liquids are usually in the order of  $10^{-9} \text{ m}^2/\text{s}$ . On the other hand,  $\mathcal{D}_{AB}$  values for solids vary from  $10^{-10}$  to  $10^{-14} \text{ m}^2/\text{s}$ .

**Example 2.3** Air at atmospheric pressure and  $95^\circ\text{C}$  flows at  $20 \text{ m/s}$  over a flat plate of naphthalene  $80 \text{ cm}$  long in the direction of flow and  $60 \text{ cm}$  wide. Experimental measurements report the molar concentration of naphthalene in the air,  $c_A$ , as a function of distance  $x$  from the plate as follows:

$x$ (cm)	$c_A$ (mol/m <sup>3</sup> )
0	0.117
10	0.093
20	0.076
30	0.063
40	0.051
50	0.043

Determine the molar flux of naphthalene from the plate surface under steady conditions.

### Solution

#### Physical properties

Diffusion coefficient of naphthalene ( $A$ ) in air ( $B$ ) at 95 °C (368 K) is

$$(\mathcal{D}_{AB})_{368} = (\mathcal{D}_{AB})_{300} \left( \frac{368}{300} \right)^{3/2} = (0.62 \times 10^{-5}) \left( \frac{368}{300} \right)^{3/2} = 0.84 \times 10^{-5} \text{ m}^2/\text{s}$$

#### Assumptions

1. The total molar concentration,  $c$ , is constant.
2. Naphthalene plate is also at a temperature of 95 °C.

#### Analysis

The molar flux of naphthalene transferred from the plate surface to the flowing stream is determined from

$$J_{Ax}^* \Big|_{x=0} = -\mathcal{D}_{AB} \left( \frac{dc_A}{dx} \right)_{x=0} \quad (1)$$

It is possible to calculate the concentration gradient on the surface of the plate by using one of the several methods explained in Section A.5 in Appendix A.

#### Graphical method

The plot of  $c_A$  versus  $x$  is given in Figure 2.5. The slope of the tangent to the curve at  $x = 0$  is  $-0.0023 \text{ (mol/m}^3\text{)/cm}$ .

#### Curve fitting method

From semi-log plot of  $c_A$  versus  $x$ , shown in Figure 2.6, it appears that a straight line represents the data fairly well. The equation of this line can be determined by the method of least squares in the form

$$y = mx + b \quad (2)$$

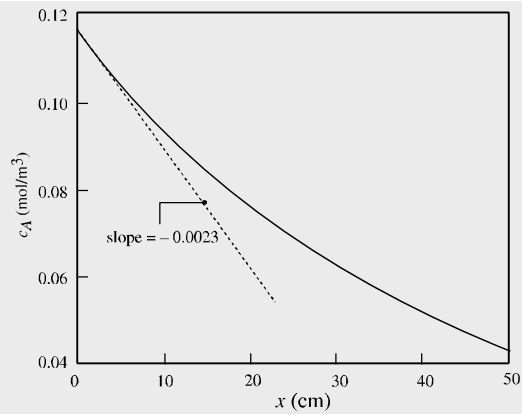


Figure 2.5. Concentration of species  $\mathcal{A}$  as a function of position.

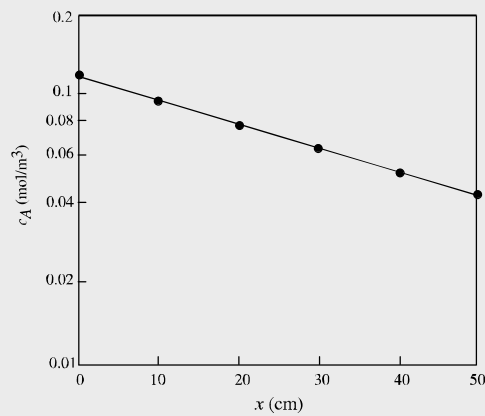


Figure 2.6. Concentration of species  $\mathcal{A}$  as a function of position.

where

$$y = \log c_A \quad (3)$$

To determine the values of  $m$  and  $b$  from Eqs. (A.6-10) and (A.6-11) in Appendix A, the required values are calculated as follows:

$y_i$	$x_i$	$x_i y_i$	$x_i^2$
-0.932	0	0	0
-1.032	10	-10.32	100
-1.119	20	-22.38	400
-1.201	30	-36.03	900
-1.292	40	-51.68	1600
-1.367	50	-68.35	2500
$\sum y_i = -6.943$	$\sum x_i = 150$	$\sum x_i y_i = -188.76$	$\sum x_i^2 = 5500$



The values of  $m$  and  $b$  are

$$m = \frac{(6)(-188.76) - (150)(-6.943)}{(6)(5500) - (150)^2} = -0.0087$$

$$b = \frac{(-6.943)(5500) - (150)(-188.76)}{(6)(5500) - (150)^2} = -0.94$$

Therefore, Eq. (2) takes the form

$$\log c_A = -0.087x - 0.94 \quad \Rightarrow \quad c_A = 0.115e^{-0.02x} \quad (4)$$

Differentiation of Eq. (4) gives the concentration gradient on the surface of the plate as

$$\left( \frac{dc_A}{dx} \right)_{x=0} = -(0.115)(0.02) = -0.0023 \text{ (mol/m}^3\text{)}/\text{cm} = -0.23 \text{ mol/m}^4$$

Substitution of the numerical values into Eq. (1) gives the molar flux of naphthalene from the surface as

$$J_{A_x}^* \Big|_{x=0} = (0.84 \times 10^{-5})(0.23) = 19.32 \times 10^{-7} \text{ mol/m}^2 \cdot \text{s}$$

## 2.2 DIMENSIONLESS NUMBERS

Newton's "law" of viscosity, Fourier's "law" of heat conduction, and Fick's first "law" of diffusion, in reality, **are not laws** but defining equations for viscosity,  $\mu$ , thermal conductivity,  $k$ , and diffusion coefficient,  $\mathcal{D}_{AB}$ . The fluxes ( $\tau_{yx}$ ,  $q_y$ ,  $j_{A_y}$ ) and the gradients ( $dv_x/dy$ ,  $dT/dy$ ,  $d\rho_A/dy$ ) must be known or measurable for the experimental determination of  $\mu$ ,  $k$ , and  $\mathcal{D}_{AB}$ .

Newton's law of viscosity, Eq. (2.1-2), Fourier's law of heat conduction, Eq. (2.1-4), and Fick's first law of diffusion, Eqs. (2.1-7) and (2.1-9), can be generalized as

$$\boxed{\left( \begin{array}{c} \text{Molecular} \\ \text{flux} \end{array} \right) = \left( \begin{array}{c} \text{Transport} \\ \text{property} \end{array} \right) \left( \begin{array}{c} \text{Gradient of} \\ \text{driving force} \end{array} \right)} \quad (2.2-1)$$

Although the constitutive equations are similar, they are not completely analogous because the transport properties ( $\mu$ ,  $k$ ,  $\mathcal{D}_{AB}$ ) have different units. These equations can also be expressed in the following forms:

$$\tau_{yx} = -\frac{\mu}{\rho} \frac{d}{dy} (\rho v_x) \quad \rho = \text{constant} \quad \rho v_x = \text{momentum/volume} \quad (2.2-2)$$

$$q_y = -\frac{k}{\rho \hat{C}_P} \frac{d}{dy} (\rho \hat{C}_P T) \quad \rho \hat{C}_P = \text{constant} \quad \rho \hat{C}_P T = \text{energy/volume} \quad (2.2-3)$$

$$j_{A_y} = -\mathcal{D}_{AB} \frac{d\rho_A}{dy} \quad \rho = \text{constant} \quad \rho_A = \text{mass of } \mathcal{A}/\text{volume} \quad (2.2-4)$$

The term  $\mu/\rho$  in Eq. (2.2-2) is called *momentum diffusivity* or *kinematic viscosity*, and the term  $k/\rho \hat{C}_P$  in Eq. (2.2-3) is called *thermal diffusivity*. Momentum and thermal diffusivities

**Table 2.1.** Analogous terms in constitutive equations for momentum, energy, and mass (or mole) transfer in one-dimension

	Momentum	Energy	Mass	Mole
Molecular flux	$\tau_{yx}$	$q_y$	$j_{A_y}$	$J_{A_y}^*$
Transport property	$\mu$	$k$	$\mathcal{D}_{AB}$	$\mathcal{D}_{AB}$
Gradient of driving force	$\frac{dv_x}{dy}$	$\frac{dT}{dy}$	$\frac{d\rho_A}{dy}$	$\frac{dc_A}{dy}$
Diffusivity	$\nu$	$\alpha$	$\mathcal{D}_{AB}$	$\mathcal{D}_{AB}$
Quantity/Volume	$\rho v_x$	$\rho \widehat{C}_P T$	$\rho_A$	$c_A$
Gradient of Quantity/Volume	$\frac{d(\rho v_x)}{dy}$	$\frac{d(\rho \widehat{C}_P T)}{dy}$	$\frac{d\rho_A}{dy}$	$\frac{dc_A}{dy}$

are designated by  $\nu$  and  $\alpha$ , respectively. Note that the terms  $\nu$ ,  $\alpha$ , and  $\mathcal{D}_{AB}$  all have the same units,  $\text{m}^2/\text{s}$ , and Eqs. (2.2-2)–(2.2-4) can be expressed in the general form as

$$\boxed{\left( \begin{array}{c} \text{Molecular} \\ \text{flux} \end{array} \right) = (\text{Diffusivity}) \left( \begin{array}{c} \text{Gradient of} \\ \text{Quantity/Volume} \end{array} \right)} \quad (2.2-5)$$

The quantities that appear in Eqs. (2.2-1) and (2.2-5) are summarized in Table 2.1.

Since the terms  $\nu$ ,  $\alpha$ , and  $\mathcal{D}_{AB}$  all have the same units, the ratio of any two of these diffusivities results in a dimensionless number. For example, the ratio of momentum diffusivity to thermal diffusivity gives the *Prandtl number*,  $\text{Pr}$ :

$$\text{Prandtl number} = \text{Pr} = \frac{\nu}{\alpha} = \frac{\widehat{C}_P \mu}{k} \quad (2.2-6)$$

The Prandtl number is a function of temperature and pressure. However, its dependence on temperature, at least for liquids, is much stronger. The order of magnitude of the Prandtl number for gases and liquids can be estimated as

$$\text{Pr} = \frac{(10^3)(10^{-5})}{10^{-2}} = 1 \quad \text{for gases}$$

$$\text{Pr} = \frac{(10^3)(10^{-3})}{10^{-1}} = 10 \quad \text{for liquids}$$

The *Schmidt number* is defined as the ratio of the momentum to mass diffusivities:

$$\text{Schmidt number} = \text{Sc} = \frac{\nu}{\mathcal{D}_{AB}} = \frac{\mu}{\rho \mathcal{D}_{AB}} \quad (2.2-7)$$

The order of magnitude of the Schmidt number for gases and liquids can be estimated as

$$\text{Sc} = \frac{10^{-5}}{(1)(10^{-5})} = 1 \quad \text{for gases}$$

$$\text{Sc} = \frac{10^{-3}}{(10^3)(10^{-9})} = 10^3 \quad \text{for liquids}$$

Finally, the ratio of  $\alpha$  to  $\mathcal{D}_{AB}$  gives the *Lewis number*,  $Le$ :

$$\text{Lewis number} = Le = \frac{\alpha}{\mathcal{D}_{AB}} = \frac{k}{\rho \widehat{C}_P \mathcal{D}_{AB}} = \frac{Sc}{Pr} \quad (2.2-8)$$

### 2.3 CONVECTIVE TRANSPORT

Convective flux or bulk flux of a quantity is expressed as

$$\left( \begin{array}{c} \text{Convective} \\ \text{flux} \end{array} \right) = (\text{Quantity/Volume}) \left( \begin{array}{c} \text{Characteristic} \\ \text{velocity} \end{array} \right) \quad (2.3-1)$$

When air is pumped through a pipe, it is considered a single phase and a single component system. In this case, there is no ambiguity in defining the characteristic velocity. However, if the oxygen in the air were reacting, then the fact that air is composed predominantly of two species,  $O_2$  and  $N_2$ , would have to be taken into account. Hence, air should be considered a single phase, binary component system. For a single phase system composed of  $n$  components, the general definition of a characteristic velocity is given by

$$v_{ch} = \sum_i^n \beta_i v_i \quad (2.3-2)$$

where  $\beta_i$  is the weighting factor and  $v_i$  is the velocity of a constituent. The three most common characteristic velocities are listed in Table 2.2. The term  $\bar{V}_i$  in the definition of the volume average velocity represents the partial molar volume of a constituent. The molar average velocity is equal to the volume average velocity when the total molar concentration,  $c$ , is constant. On the other hand, the mass average velocity is equal to the volume average velocity when the total mass density,  $\rho$ , is constant.

The choice of a characteristic velocity is arbitrary. For a given problem, it is more convenient to select a characteristic velocity that will make the convective flux zero and thus yield a simpler problem. In the literature, it is common practice to use the molar average velocity for dilute gases, i.e.,  $c = \text{constant}$ , and the mass average velocity for liquids, i.e.,  $\rho = \text{constant}$ .

It should be noted that the molecular mass flux expression given by Eq. (2.1-6) represents the molecular mass flux with respect to the mass average velocity. Therefore, in the equation representing the total mass flux, the characteristic velocity in the convective mass flux term is taken as the mass average velocity. On the other hand, Eq. (2.1-8) is the molecular molar flux with respect to the molar average velocity. Therefore, the molar average velocity is considered the characteristic velocity in the convective molar flux term.

**Table 2.2.** Common characteristic velocities

Characteristic Velocity	Weighting Factor	Formulation
Mass average	Mass fraction ( $\omega_i$ )	$v = \sum_i \omega_i v_i$
Molar average	Mole fraction ( $x_i$ )	$v^* = \sum_i x_i v_i$
Volume average	Volume fraction ( $c_i \bar{V}_i$ )	$v^{\blacksquare} = \sum_i c_i \bar{V}_i v_i$

## 2.4 TOTAL FLUX

Since the total flux of any quantity is the sum of its molecular and convective fluxes, then

$$\left( \begin{array}{c} \text{Total} \\ \text{flux} \end{array} \right) = \underbrace{\left( \begin{array}{c} \text{Transport} \\ \text{property} \end{array} \right) \left( \begin{array}{c} \text{Gradient of} \\ \text{driving force} \end{array} \right)}_{\text{Molecular flux}} + \underbrace{\left( \begin{array}{c} \text{Quantity} \\ \text{Volume} \end{array} \right) \left( \begin{array}{c} \text{Characteristic} \\ \text{velocity} \end{array} \right)}_{\text{Convective flux}} \quad (2.4-1)$$

or,

$$\left( \begin{array}{c} \text{Total} \\ \text{flux} \end{array} \right) = \underbrace{(\text{Diffusivity}) \left( \begin{array}{c} \text{Gradient of} \\ \text{Quantity/Volume} \end{array} \right)}_{\text{Molecular flux}} + \underbrace{\left( \begin{array}{c} \text{Quantity} \\ \text{Volume} \end{array} \right) \left( \begin{array}{c} \text{Characteristic} \\ \text{velocity} \end{array} \right)}_{\text{Convective flux}} \quad (2.4-2)$$

The quantities that appear in Eqs. (2.4-1) and (2.4-2) are given in Table 2.3.

The general flux expressions for momentum, energy, and mass transport in different coordinate systems are given in Appendix C.

From Eq. (2.4-2), the ratio of the convective flux to the molecular flux is given by

$$\frac{\text{Convective flux}}{\text{Molecular flux}} = \frac{(\text{Quantity/Volume})(\text{Characteristic velocity})}{(\text{Diffusivity})(\text{Gradient of Quantity/Volume})} \quad (2.4-3)$$

**Table 2.3.** Analogous terms in flux expressions for various types of transport in one-dimension

Type of Transport	Total Flux	Molecular Flux	Convective Flux	Constraint
Momentum	$\pi_{yx}$	$-\mu \frac{dv_x}{dy}$	$(\rho v_x) v_y$	None
		$-v \frac{d(\rho v_x)}{dy}$		$\rho = \text{const.}$
Energy	$e_y$	$-k \frac{dT}{dy}$	$(\rho \hat{C}_P T) v_y$	None
		$-\alpha \frac{d(\rho \hat{C}_P T)}{dy}$		$\rho \hat{C}_P = \text{const.}$
Mass	$\mathcal{W}_{Ay}$	$-\rho \mathcal{D}_{AB} \frac{d\omega_A}{dy}$	$\rho_A v_y$	None
		$-\mathcal{D}_{AB} \frac{d\rho_A}{dy}$		$\rho = \text{const.}$
Mole	$N_{Ay}$	$-c \mathcal{D}_{AB} \frac{dx_A}{dy}$	$c_A v_y^*$	None
		$-\mathcal{D}_{AB} \frac{dc_A}{dy}$		$c = \text{const.}$

Since the gradient of a quantity represents the variation of that particular quantity over a characteristic length, the “Gradient of Quantity/Volume” can be expressed as

$$\text{Gradient of Quantity/Volume} = \frac{\text{Difference in Quantity/Volume}}{\text{Characteristic length}} \quad (2.4-4)$$

The use of Eq. (2.4-4) in Eq. (2.4-3) gives

$$\frac{\text{Convective flux}}{\text{Molecular flux}} = \frac{(\text{Characteristic velocity})(\text{Characteristic length})}{\text{Diffusivity}} \quad (2.4-5)$$

The ratio of the convective flux to the molecular flux is known as the *Peclet number*,  $Pe$ . Therefore, Peclet numbers for heat and mass transfers are

$$Pe_H = \frac{v_{ch} L_{ch}}{\alpha} \quad (2.4-6)$$

$$Pe_M = \frac{v_{ch} L_{ch}}{\mathcal{D}_{AB}} \quad (2.4-7)$$

Hence, the total flux of any quantity is given by

$$\text{Total flux} = \begin{cases} \text{Molecular flux} & Pe \ll 1 \\ \text{Molecular flux} + \text{Convective flux} & Pe \simeq 1 \\ \text{Convective flux} & Pe \gg 1 \end{cases} \quad (2.4-8)$$

#### 2.4.1 Rate of Mass Entering and/or Leaving the System

The mass flow rate of species  $i$  entering and/or leaving the system,  $\dot{m}_i$ , is expressed as

$$\dot{m}_i = \left[ \underbrace{\left( \frac{\text{Mass}}{\text{Diffusivity}} \right) \left( \frac{\text{Gradient of Mass of } i/\text{Volume}}{\text{Mass of } i/\text{Volume}} \right)}_{\text{Molecular mass flux of species } i} + \underbrace{\left( \frac{\text{Mass of } i}{\text{Volume}} \right) \left( \frac{\text{Characteristic velocity}}{\text{velocity}} \right)}_{\text{Convective mass flux of species } i} \right] \left( \frac{\text{Flow}}{\text{area}} \right) \quad (2.4-9)$$

In general, the mass of species  $i$  may enter and/or leave the system by two means:

- Entering and/or leaving conduits,
- Exchange of mass between the system and its surroundings through the boundaries of the system, i.e., interphase transport.

When a mass of species  $i$  enters and/or leaves the system by a conduit(s), the characteristic velocity is taken as the average velocity of the flowing stream and it is usually large enough to neglect the molecular flux compared to the convective flux, i.e.,  $Pe_M \gg 1$ . Therefore, Eq. (2.4-9) simplifies to

$$\dot{m}_i = \left( \frac{\text{Mass of } i}{\text{Volume}} \right) \left( \frac{\text{Average}}{\text{velocity}} \right) \left( \frac{\text{Flow}}{\text{area}} \right) \quad (2.4-10)$$

or,

$$\boxed{\dot{m}_i = \rho_i \langle v \rangle A = \rho_i Q} \quad (2.4-11)$$

Summation of Eq. (2.4-11) over all species leads to the total mass flow rate,  $\dot{m}$ , entering and/or leaving the system by a conduit in the form

$$\dot{m} = \rho \langle v \rangle A = \rho Q \quad (2.4-12)$$

On a molar basis, Eqs. (2.4-11) and (2.4-12) take the form

$$\dot{n}_i = c_i \langle v \rangle A = c_i Q \quad (2.4-13)$$

$$\dot{n} = c \langle v \rangle A = c Q \quad (2.4-14)$$

On the other hand, when a mass of species  $i$  enters and/or leaves the system as a result of interphase transport, the flux expression to be used is dictated by the value of the Peclet number as shown in Eq. (2.4-8).

## 2.4.2 Rate of Energy Entering and/or Leaving the System

The rate of energy entering and/or leaving the system,  $\dot{E}$ , is expressed as

$$\dot{E} = \left[ \underbrace{\left( \frac{\text{Thermal diffusivity}}{\text{Energy/Volume}} \right) \left( \frac{\text{Gradient of Energy/Volume}}{\text{Energy/Volume}} \right)}_{\text{Molecular energy flux}} + \underbrace{\left( \frac{\text{Energy}}{\text{Volume}} \right) \left( \frac{\text{Characteristic velocity}}{\text{Energy/Volume}} \right)}_{\text{Convective energy flux}} \right] \left( \frac{\text{Flow}}{\text{area}} \right) \quad (2.4-15)$$

As in the case of mass, energy may enter or leave the system by two means:

- By inlet and/or outlet streams,
- By exchange of energy between the system and its surroundings through the boundaries of the system in the form of heat and work.

When energy enters and/or leaves the system by a conduit(s), the characteristic velocity is taken as the average velocity of the flowing stream and it is usually large enough to neglect the molecular flux compared to the convective flux, i.e.,  $Pe_H \gg 1$ . Therefore, Eq. (2.4-15) simplifies to

$$\dot{E} = \left( \frac{\text{Energy}}{\text{Volume}} \right) \left( \frac{\text{Average}}{\text{velocity}} \right) \left( \frac{\text{Flow}}{\text{area}} \right) \quad (2.4-16)$$

Energy per unit volume, on the other hand, is expressed as the product of energy per unit mass,  $\hat{E}$ , and mass per unit volume, i.e., density, such that Eq. (2.4-16) becomes

$$\dot{E} = \left( \frac{\text{Energy}}{\text{Mass}} \right) \underbrace{\left( \frac{\text{Mass}}{\text{Volume}} \right) \left( \frac{\text{Average}}{\text{velocity}} \right) \left( \frac{\text{Flow}}{\text{area}} \right)}_{\text{Mass flow rate}} = \hat{E} \dot{m} \quad (2.4-17)$$

## PROBLEMS

2.2. A Newtonian fluid with a viscosity of 50 cP is placed between two large parallel plates separated by a distance of 8 mm. Each plate has an area of  $2 \text{ m}^2$ . The upper plate moves in the positive x-direction with a velocity of 0.4 m/s while the lower plate is kept stationary. (a) Calculate the steady force applied to the upper plate. (b) The fluid in part (a) is replaced with another Newtonian fluid of viscosity 5 cP. If the steady force applied to the upper plate is the same as that of part (a), calculate the velocity of the upper plate.

Diagram showing two parallel plates separated by a distance of 8 mm. The upper plate moves with a velocity of 0.4 m/s in the positive x-direction. The fluid between the plates is labeled 'FLUID'.

Equation for shear stress:

$$\tau_{yx} = \mu \frac{dv_x}{dy}$$

Equation for shear force:

$$\tau_{yx} = \frac{F}{A} = \frac{(50 \times 10^{-3}) \text{ kg}}{\text{m} \cdot \text{s}} \times \frac{0.4 \text{ m}}{8 \times 10^{-3} \text{ s} \cdot \text{m}}$$

Calculation for force:

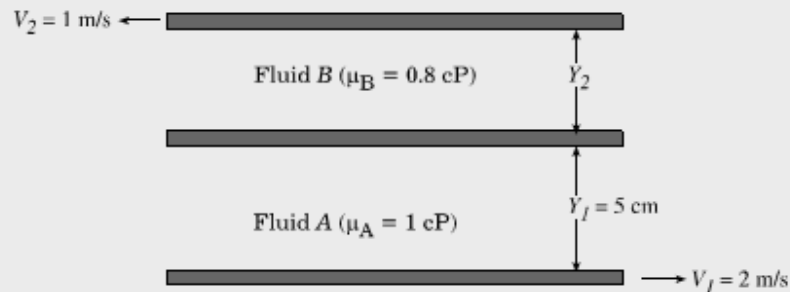
$$\frac{F}{A} = 2.5 \frac{\text{kg}}{\text{m}}$$
$$F = 2.5 \frac{\text{kg}}{\text{m}} \times 2 \text{ m}^2$$
$$\Rightarrow 5 \frac{\text{kg} \cdot \text{m}}{\text{s}^2} = 5 \text{ N}$$

Assuming  $F$  to be constant; 5 N.

Calculation for velocity:

$$\mu = 5 \text{ cP} = 5 \times 10^{-3} \text{ kg/m} \cdot \text{s}$$
$$\frac{F}{A} = \mu \frac{v}{y}$$
$$\frac{5}{2} = 5 \times 10^{-3} \times \frac{v}{0.008}$$
$$\therefore v = 4 \text{ m/s}$$

2.3 Three parallel flat plates are separated by two fluids as shown in the figure below. What should be the value of  $Y_2$  so as to keep the plate in the middle stationary?



(Answer: 2 cm)

**Answer:**  $F/A = -\mu_A \frac{V_1}{Y_1} = -1 \times 10^{-3} \times \frac{2}{5 \times 10^{-2}} = -4 \text{ N}$   
 Now,  $4 = 0.8 \times 10^{-3} \times \frac{1}{Y_2 \times 10^{-2}}$   
 $Y_2 = 0.02 \text{ m} = 2 \text{ cm}$

2.4 The steady rate of heat loss through a plane slab, which has a surface area of  $3 \text{ m}^2$  and is  $7 \text{ cm}$  thick, is  $72 \text{ W}$ . Determine the thermal conductivity of the slab if the temperature distribution in the slab is given as

$$T = 5x + 10$$

where  $T$  is temperature in  $^\circ\text{C}$  and  $x$  is the distance measured from one side of the slab in  $\text{cm}$ .

(Answer:  $0.048 \text{ W/m}\cdot\text{K}$ )

Energy Flux =  $\frac{Q}{A} = \frac{72 \text{ W}}{3 \text{ m}^2} = 24 \frac{\text{W}}{\text{m}^2}$

Given, distribution  $T = 5x + 10$  differentiating w.r.t to  $x$

$$\frac{dT}{dx} = 5 \frac{\text{K}}{\text{cm}} = 5 \frac{\text{K}}{10^{-2} \text{ m}} = 500 \frac{\text{K}}{\text{m}}$$

Substituting in equation (1)

$$24 \frac{\text{W}}{\text{m}^2} = +K \cdot \left( 500 \frac{\text{K}}{\text{m}} \right)$$

$K = 0.048 \frac{\text{W}}{\text{m}\cdot\text{K}}$  (-ve indicates  $\downarrow$  intemp)



2.5 The inner and outer surface temperatures of a 20 cm thick brick wall are 30°C and -5°C, respectively. The surface area of the wall is 25 m<sup>2</sup>. Determine the steady rate of heat loss through the wall if the thermal conductivity is 0.72 W/m·K.

(Answer: 3150 W)

$k = 0.72 \text{ W/(m}\cdot\text{K)}$   
 $A = 25 \text{ m}^2$   
 $20 \text{ cm}$   
 $30^\circ\text{C}$   
 $-5^\circ\text{C}$

$$Q = ? \quad -kAd \frac{T}{dr}$$

$$= -0.72 \times \frac{-5 - 30}{20 \times 10^{-2}}$$

$$= -0.72 \times 25 \times \frac{-35}{20 \times 10^{-2}}$$

$Q = 3150 \text{ W}$

2.12 Air at 20°C and 1 atm pressure flows over a porous plate that is soaked in ethanol. The molar concentration of ethanol in the air,  $c_A$ , is given by

$$c_A = 4e^{-1.5z}$$

where  $c_A$  is in kmol/m<sup>3</sup> and  $z$  is the distance measured from the surface of the plate in meters. Calculate the molar flux of ethanol from the plate.

(Answer: 0.283 kmol/m<sup>2</sup>·h)

2.10  $T = 20^\circ\text{C}$ , 1 atm,  $c_A = 4e^{-1.5z}$ ,  $J_A = -D_{AB} \frac{dc_A}{dz}$   
 $\frac{dc_A}{dz} = 4 \frac{d e^{-1.5z}}{dz}$   
 $\frac{dc_A}{dz} = 4(-1.5) e^{-1.5z}$   
 $\left. \frac{dc_A}{dz} \right|_{z=0} = -6.0 \text{ kmol/m}^3$

$\frac{0.283 \text{ mol/m}^3 \cdot 3600 \text{ s}}{6} = 13.6 \times 10^{-6} \text{ mol/s}$   
 $\frac{0.283}{6 \times 3600} = 0.283 \frac{\text{kmol}}{\text{m}^2 \cdot \text{h}}$

$J_A \Big|_{z=0} = -D_{AB} \times -6 \text{ mol/(m}\cdot\text{s)}$   
 $= 1.31 \times 10^{-5} \times -6 z$   
 at 313 =  $1.45 \times 10^{-5}$   
 $(D_{AB})_{\text{Ethanol}}$   
 $(D_{AB})_{\text{Ethanol at 293}} = 1.45 \times 10^{-5} \left( \frac{293}{313} \right)^{3/2}$   
 $= 1.31 \times 10^{-5} \text{ m}^2/\text{s}$