

SCHOOL OF BIO & CHEMICAL ENGINEERING

DEPARTMENT OF CHEMICAL ENGINEERING

UNIT – I – Transport Phenomena for Bioprocesses – SCHA1511

Unit I Momentum Transport

Introduction to Momentum Transport

Momentum transport deals with the transport of momentum which is responsible for flow in fluids. Momentum transport describes the science of fluid flow also called fluid dynamics. A few basic assumptions are involved in fluid flow and these are discussed below. No slip boundary condition This is the first basic assumption used in momentum transport. It deals with the fluid flowing over a solid surface, and states that whenever a fluid comes in contact with any solid boundary, the adjacent layer of the fluid in contact with the solid surface has the same velocity as the solid surface. Hence, we assumed that there is no slip between the solid surface and the fluid or the relative velocity is zero at the fluid–solid interface. For example, consider a fluid flowing inside a stationary tube of radius *R* as shown in Fig 7.1. Since the wall of the tube at r=R is stationary, according to the no-slip condition implies that the fluid velocity at r=R is also zero.



Fig .1 Fluid flow in a circular tube of radius R

In the second example as shown in Fig .2, there are two plates which are



separated by a Fig .2 Fig. 2 Two parallel plates at stationary condition distance h, and some fluid is present between these plates. If the lower plate is forced to move with a velocity V in x direction and the upper plate is held stationary, no-slip boundary conditions may be written as follows.

Thus, for Re <2100, we have laminar flow, i.e., no mixing in the radial direction leading to a thread like flow and for $\mathbf{R}e >2100$, we have the turbulent flow, i.e., mixing in the radial direction between layers of fluid.

In laminar flow, the fluid flows as a stream line flow with no mixing between layers. In turbulent flow, the fluid is unstable and mixes rapidly due to fluctuations and disturbances in the flow. The disturbance might be present due to pumps, friction of the solid surface or any type of noise present in the system. This makes solving fluid flow problem much more difficult. To understand the difference in the velocity profile in two kinds of fluid flows, we consider a fluid flowing to a horizontal tube in z direction under steady state condition. Then, we can intuitively see the velocity profile may be shown below.

Fluid:

A fluid is a gas or liquid that, unlike a solid, flows to assume the shape of the container in which it is placed. This occurs because a fluid responds to a shear stress, or a force per unit area directed along the face of a cube of fluid, by flowing, rather than by an elastic displacement as in a solid.

TYPES OF FLUIDS BASED ON VISCOSITY:

The fluids may be classified into following five types:

- 1. Ideal fluid
- 2. Real fluid
- 3. Newtonian fluid
- 4. Non-Newtonian fluid
- 5. Ideal plastic fluid

Properties of fluid

Density: Density of a fluid is defined as the ratio of the mass of a fluid to its volume.

Specific Volume: Specific volume of a fluid is defined as the volume of a fluid occupied by a unit mass or volume per unit mass of a fluid.

Viscosity of liquid: Viscosity is defined as the property of a fluid which offers resistance to the movement of one layer of fluid over another adjacent layer of fluid.

$$y = 0, v_x = v$$
$$y = H, v_x = 0$$

Thus, every layer of fluid is moving at a different velocity. This leads to shear forces which are described in the next section.

Newton's Law of Viscosity

Newton's law of viscosity may be used for solying problem for Newtonian fluids. For many fluids in chemical engineering the assumption of Newtonian fluid is reasonably acceptable. To understand Newtonian fluid, let us consider a hypothetical experiment, in which there are two infinitely large plates situated parallel to each other, separated by a distance h. A fluid is present between these two plates and the contact area between the fluid and the plates is A.

A constant force *F1* is now applied on the lower plate while the upper plate is held stationary. After steady state has reached, the velocity achieved by the lower plate is measured as V_l . The force is then changed, and the new velocity of the plate associated with this force is measured. The experiment is then repeated to take sufficiently large readings as shown in the following table. Table 1. Applied force vs velocity

-**1**-- 0

$$\frac{F}{A} \propto \frac{dv_x}{dy}$$
$$\frac{F}{A} = \pm \mu \frac{dv_x}{dy}$$

surface on which this force is acting. The quantity or the velocity gradient is also called the shear rate. μ is a property of the fluid and is measured the resistance offered by the fluid to flow. Viscosity may be constant for many Newtonian fluids and may change only with temperature.

Thus, the Newton's law of viscosity, in its most basic form is given as

The shear stress is directly proportional to velocity gradient. The constant of proportionality is known as coefficient of viscosity.

Variation of viscosity with respect to temperature

Viscosity of fluids is due to

1. cohesion between the fluid molecules and

2. transfer of momentum between the molecules.

Fluids are aggregations of molecules; widely spaced for a gas and closely spaced for liquids. Distance between the molecules is very large compared to the molecular diameter. The number of molecules involved is immense and the separation between them is normally negligible. Under these conditions, fluid can be treated as continuum and the properties at any point can be treated as bulk behavior of the fluids. For the continuum model to be valid, the smallest sample of matter of practical interest must contain a large number of molecules so that meaningful averages can be calculated. In the case of air at sea-level conditions, a volume of 10⁻⁹ mm³ contains 3×10⁷ molecules. In engineering sense, this volume is quite small, so the continuum hypothesis is valid. 4

If the F/A is plotted against V/h, we may observe that they lie on a straight line passing through the origin.



Fig 4 Shear stress vs. shear stain

Thus, it may be said that F/A is proportional to v/h for a Newtonian fluid.

$$\frac{F}{A} \propto \frac{v}{h}$$

It may be noted that it is the velocity gradient which leads to the development of shear forces. The above equation may be re-written as

$$\Rightarrow \frac{F_1}{A} \propto \frac{v_1 - 0}{h - 0} = \frac{\Delta v_x}{\Delta y}$$

In the limiting case, as $h \rightarrow 0$, we have

where, μ is a constant of proportionality, and is called as the viscosity of the fluid. The quantity

F/A represents the shear forces/stress. It may be represented as τ_{yx} , where the subscript *x* indicates the direction of force and subscript *y* indicates the direction of outward normal of the

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

Newton's law of viscosity states that the shear stress is directly proportional to Velocity gradient.

Here, both '+' or '-' sign are valid. The positive sign is used in many fluid mechanics books whereas the negative sign may be found in transport

phenomena books. If the positive sign is used then τ_{yx} may be called the

shear force while if the negative sign is used τ_{yx} may be referred to as the momentum flux which flows from a higher value to a lower value.

$$\tau_{yx} = +\mu \frac{dv_x}{dy} \rightarrow \text{Shear force}$$

 $\tau_{yx} = -\mu \frac{dv_x}{dy} \rightarrow \text{Momentum flux}$

The reason for having a negative sign for momentum flux in the transport phenomena is to have similarities with Fourier's law of heat conduction in heat transport and Ficks law of diffusion in mass transport. For example, in heat transport, heat flows from higher temperature to lower temperature indicating that heat flux is positive when the temperature gradient is negative. Thus, a minus sign is required in the Fourier's law of heat

conduction. The interpretation of τ_{yx} as the momentum flux is that x directed momentum flows from higher value to lower value in y direction.

Viscosity

Viscosity is a measure of flow resistance to the fluid. The viscosity is of two types dynamic or absolute viscosity and kinematic viscosity. Dynamic viscosity is simply the viscosity offered as resistance to fluid flow. Kinematic viscosity is defined as the ratio of absolute viscosity to density.

$$\mu = \frac{Force/Area}{\left[\frac{dv_x}{dy}\right]} = \frac{MLT^{-1}L^{-2}}{LT^{-1}L^{-1}} = ML^{-1}T^{-1}$$

The SI unit of viscosity is kg/m.s or Pa.s. In CGS unit is g/cm.s and is commonly known as poise (*P*). where 1 P = 0.1 kg/m.s. The unit poise is also used with the prefix *centi*-, which refers to one-hundredth of a poise, i.e. 1cP = 0.01 P. The viscosity of air at $25^{\circ}C$ is 0.018 cP, water at $25^{\circ}C$ is 1 cP and for many polymer melts it may range from 1000 to 100,000 cP, thus showing a long range of viscosity.

Laminar and turbulent flow

Fluid flow can broadly be categorized into two kinds: laminar and turbulent. In laminar flow, the fluid layers do not inter-mix, and flow separately. This is the flow encountered when a tap is just opened and water is allowed to flow very slowly. As the flow increases, it becomes much more irregular and the different fluid layers start mixing with each other leading to turbulent flow. Osborne Reynolds tried to distinguish between the two kinds of flow using an ingenious experiment and known as the Reynolds's experiment. The basic idea behind this experiment is described below.

The experiment setup used for performing the Reynolds's experiment is shown in Fig. 7.5. The average velocity of fluid flow through the pipe diameter can be varied. Also, there is an arrangement to inject a colored dye at the center of the pipe. The profile of the dye is observed along the length of the pipe for different velocities for different fluids. If this experiment is performed, it may be seen that for certain cases the dye shows a regular thread type profile, which is seen at low fluid velocity and flow is called laminar flow. when the fluid velocity is increased the dye starts to mixed with the fluid and for larger velocities simply disappears. At this point fluid flow becomes turbulent.

For the variables average velocity of fluid $v_z avg$, pipe diameter *D*, fluid density ρ , and the fluid viscosity μ , Reynolds found a dimensionless group which could be used to characterize the type of fluid flow in the tube. This dimensionless quantity is known as the Reynolds number. From the experiment, It was observed that if Re > 2100, the dye simply disappeared and the flow has changed to laminar to turbulent flow.

For laminar flow, it is observed that fluid flows as smooth stream line and all other components of velocity are zero. Thus

$$v_z = v_z(r)$$
$$v_r = 0$$
$$v_\theta = 0$$

For turbulent flow, if we observe the fluid flows at a local point. It is observed that fluid flows in very random manner in all directions where these local velocities may be the function of any dimensions.

$$v_{z} = v_{z}(r, z, \theta, t)$$
$$v_{r} = v_{r}(r, z, \theta, t)$$
$$v_{\theta} = v_{\theta}(r, z, \theta, t)$$

Internal and external flows

Depending on how the fluid and the solid boundaries contact each other, the flow may be classified as internal flow or external flow. In internal flows, the fluid moves between solid boundaries as is the case when fluid flows in a pipe or a duct. In external flows, however, the fluid is flowing over an external solid surface, the example may be sited is the flow of fluid over a sphere as shown in Fig. 8.1.

On the other hand, if the velocity of fluid is very low the deviation due to disturbances may decay with time, and becomes negligible after that. Thus the flow remains in laminar region. Consider a practical example in which some cars

are moving on the highway in the same direction but in the different lanes at different speeds. If suddenly, some obstacle comes on the road, then if the car's speed is sufficiently low, it can move on to other lane smoothly and come back to its original lane after the obstacle is crossed. This is the regular laminar case. On the other hand, if the car is moving at a high speed and suddenly encounters an obstacle, then the driver may lose control, and this car may move haphazardly and hit other cars and after that traffic may never return to normal traffic conditions. This is the turbulent case.



Fig 8.1 External flow around a sphere

Boundary layers and fully developed regions Let us now consider the example of fluid flowing over a horizontal flat plate as shown in Fig.

The velocity of the fluid is before it encounters the plate. As the fluid touches the plate, the velocity of the fluid layer just adjacent to the plate surface becomes zero due to the no slip boundary condition. This layer of fluid tries to drag the next fluid layer above it and reduces its velocity. As the fluid proceeds along the length of the plate (in x-direction), each layer starts to drag adjacent fluid layer but the effect of drag reduces as we go further away from the plate in y-direction. Finally, at some distance from the plate this drag effect disappears or becomes insignificant. This region where the velocity is changing or where the velocity gradients exists, is called the boundary layer region. The region beyond boundary layer where the velocity gradients are insignificant is called the potential flow region.

Thus, we see that for laminar flow there is only one component of velocity present and it depends only on one coordinate whereas the solution of turbulent flow may be vary complex. For turbulent flow, one can ask the question that if the fluid is flowing in the z direction then why are the velocity components in r and θ direction non-zero? The mathematical answer for this question can be deciphered from the equation of motion. The equation of motion is a non-linear partial differential equation. This non-linear nature of the equation causes instability in the system which produces flow in other directions. The instability in the system may occur due to any disturbances or noise present in the environment.



Fig 8.2 External flow over a flat plate

As depicted in Fig. 8.2, the boundary layer keeps growing along the x-direction, and may be referred to as the developing flow region. In internal flows (e.g. fluid flow through a pipe), the boundary layers finally merge after flow over a distance as shown in Fig. 8.3 below.



Fig 8.3 Developing flow and fully developed flow region

The region after the point at which the layers merge is called the fully developed flow region and before this it is called the developing flow region. In fact, fully developed flow is another important assumption which is taken for finding solution for varity of fluid flow problem. In the fully developed flow region (as shown in Figure 8.3), the velocity vz is a function of r direction only. However, the developing flow region, velocity vz is also changing in the z direction.

Main axioms of transport phenomena

The basic equations of transport phenomena are derived based on following five axioms.

- Mass is conserved, which leads to the equation of continuity.
- Momentum is conserved, which leads to the equation of motion.
- Moment of momentum is conserved leads to an important result that the 2nd order

stress tensor $\tilde{~}$ is symmetric.

- Energy is conserved, which leads to equation of thermal energy.
- Mass of component i in a multi-component system is conserved, which leads to the convective diffusion equation.

The solution of equations, resulting from axiom 2, 4 and 5 leads to the solution of velocity, temperature and concentration profiles. Ones these profiles are known, all other important information needed can be determined. We first take the axiom -1. Other axioms will be taken up one by one letter on.

There are three types of control volumes (CV) which may be chosen for deriving the equations based these axioms.

• Rectangular shaped control volume fixed in space

In this case, the control volume is rectangular volume element and is fixed in space. This method is the easiest to understand but requires more number of steps.

• Irregular shaped control volume element fixed in space

In this case, the control volume can be of any shape, but it is again fixed in space. This method is somewhat more difficult than the previous method as it requires little better understanding vector analysis and surface and volume integrals.

• Material volume approach

In this case, the control volume can be of any shape but moves with the velocity of the flowing fluid. This method is most difficult in terms of mathematics, but requires least number of steps for deriving the equations.

All three approaches when applied to above axiom, lead to the same equations. In this web course, we follow the first approach. Other approaches may be found elsewhere. Axioms-1

Mass is conserved

Consider a fluid of density ρ flowing with velocity \mathcal{Y} as shown in Fig. 8.4. Here, ρ and \mathcal{Y} are functions of space (x,y,z) and time (t). For conversion of mass, the rate of mass entering and leaving from the control volume (net rate of inflow) has to be evaluated and this should be equal to the rate of accumulation of mass in the control volume (CV). Thus, conservation of mass may be written in words as given below

$$\begin{pmatrix} \text{rate of accumulation of} \\ \text{mass in control volume} \end{pmatrix} = \begin{pmatrix} \text{rate of inflow of mass} \\ \text{into control volume} \end{pmatrix} - \begin{pmatrix} \text{rate} \\ \text{out} \end{pmatrix}$$



Fig 4 Fixed rectangular volume element through which fluid is flowing

The equation is then divided by the volume of the CV and converted into a partial differential equation by taking the limit as all dimensions go to zero. This limit effectively means that CV collapses to a point, thereby making the equation valid at every point in the system.

Let m and m+ Δ m be the mass of the control volume at time t and t+ Δ t respectively. Then, the rate of accumulation,

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

In order to evaluate the rate of inflow of mass into the control volume, we need to inspect how mass enters the control volume. Since the fluid velocity has three components vx, vy and vz, we need to identify the components which cause the inflow or the outflow at each of the six faces of the rectangular CV. For example, it is the component vx which forces the fluid to flow in the x direction, and thus it makes the fluid enter or exit through the faces having area $\Delta y \Delta z$ at x = x and $x = x + \Delta x$ respectively. The component vy forces the fluid in y direction, and thus it makes the fluid to flow in z direction, and thus it makes the fluid to flow in z direction, and thus it makes the fluid to flow in z direction, and thus it makes fluid enter or exit through the faces having area $\Delta x \Delta z$ at y = y and $y = y + \Delta y$ respectively. Similarly, the component vz forces the fluid to flow in z direction, and thus it makes fluid enter or exit through the faces having area $\Delta x \Delta y$ at z = z and $z = z + \Delta z$ respectively.

The rate mass entering in x direction through the surface $\Delta y \Delta z$ is $(\rho v x \Delta y \Delta z | x)$, the rate of mass entering in y direction through the surface $\Delta x \Delta z$ is $(\rho v y \Delta x \Delta z | y)$ and the rate of mass entering from z direction through the surface $\Delta x \Delta y$ is $(\rho v z \Delta x \Delta y | z)$. In a similar manner, expressions for the rate of mass leaving from the control volume may be written.

Thus, the conservation of mass leads to the following expressions

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

Dividing the Equation (8.1) by the volume $\Delta x \Delta y \Delta z$, we obtain

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

Note that each term in Equation (8.2) has the unit of mass per unit volume per unit time. Now, taking the limits $\Delta x \rightarrow 0$, $\Delta y \rightarrow 0$ and $\Delta z \rightarrow 0$, we get

$$\frac{\partial \rho}{\partial t} = \lim_{\Delta x \to 0} \left[\frac{(\rho v_x)|_x - (\rho v_x)|_{x + \Delta x}}{\Delta x} \right] + \lim_{\Delta y \to 0} \left[\frac{(\rho v_y)|_y - (\rho v_y)|_{y + \Delta y}}{\Delta y} \right] + \lim_{\Delta z \to 0} \left[\frac{(\rho v_y)|_y - (\rho v_y)|_{y + \Delta y}}{\Delta y} \right]$$

and using the definition of derivative, we finally obtain

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

Equation (8.4) is applicable to each point of the fluid. Rearranging the terms, we get the equation of continuity, may be written as given below.

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

We need not to derive the equation of continuity again and again in other coordinate system (that is, spherical or cylindrical). The idea is to rewrite Equation (8.5) in vector and tensor form. Once it is written in this form, the same equation may be applied to other coordinate system as well. Thus, the Equation (8.5) may be rewritten in vector and tensor form as shown below.

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

Vector and tensor analysis of cylindrical and spherical coordinate systems is not done here, and can be looked up elsewhere. Thus, the final expressions in cylindrical and spherical coordinates

are given as below.

cylindrical coordinates (r, θ , z)

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

Spherical coordinates (r, θ, ϕ)

$$\frac{\partial \rho}{\partial t} + \frac{1}{r^2} \frac{\partial}{\partial r} (\rho r v_r) + \frac{1}{r \sin \theta} \frac{\partial}{\partial \theta} (\rho v_\theta \sin \theta) + \frac{1}{r \sin \theta} \frac{\partial}{\partial \varphi} (\rho v_\varphi) = 0$$

Equation of continuity in terms of substantial derivative

The second term in Equation (8.6) may be broken into two parts as shown below. Partial derivative present in the Equation (8.6) can be converted into substantial derivative using vector and tensor identities.

$$\frac{\partial \rho}{\partial t} + \underline{v}.\nabla \rho + \rho \nabla .\underline{v} = 0$$

In the above equation, the first two terms may be combined using the definition of substantial derivative to obtain the following equation.

$$\frac{D\rho}{Dt} + \rho \nabla \underline{y} = 0$$

In some cases, the fluid may be incompressible, i.e. density ρ is a constant with time as well as space coordinates. For example, water may be assumed as an incompressible fluid under isothermal conditions. In fact, all liquids may be assumed as incompressible fluids under isothermal conditions. For this special case, the equation of continuity may be further simplified as shown below

$$\nabla \underline{y} = 0$$
 (ρ is constant)

The above equation for an incompressible fluid does not mean that the system is under steady state conditions. The velocity of the fluid may still be a function of time. It only implies that if the velocity of the fluid changes in a particular direction (x, y or z) then it should also change in the other directions such that mass is conserved without changing its density. The equation of continuity provides additional information about the velocity profile and helps in solution of

Flow through circular tube

Flow of fluids through a circular tube is a common problem, encountered frequently in different fields of engineering. Consider an incompressible, Newtonian fluid, flowing through a horizontal circular tube as shown in Fig. (10.1). Assume that the fluid flow is laminar and under steady state conditions. Determine the velocity profile and average velocity of the fluid using shell momentum balance approach.

Assumptions

- Fluid density and viscosity are constants.
- System is in steady state.
- Laminar flow (simple shear flow).
- Newton's law of viscosity is applicable.
- Fully developed flow.



Fig Laminar flow in a horizontal pipe

Intuitively guess the velocity profile

Since the flow is steady and laminar, we may intuitively say that the velocities in r direction and θ direction are zero. Due to steady state conditions, the fluid velocity in z direction, vz, is not dependent on time t. Furthermore, due to the axisymmetric geometry fluid flow the velocity vz is

independent of θ . Thus,

$$v_r = 0, v_{\theta} = 0, v_z = v_z(r, Z, \mathcal{A}, \mathfrak{A})$$

 $v_z = v_z(r, z)$

By applying the equation of continuity in cylindrical coordinates

$$\frac{\partial v_z}{\partial z} = 0$$

Hence,
 $v_z = v(r)$

Since the fluid is flowing in z direction, we may conclude the following.

- Since vr=0, r directional momentum balance is not important.
- Since $v\theta=0$, θ directional momentum balance is again not important.
- Since vz≠0, z directional momentum balance is most important.

Equation for circular pipe:

The control volume should be decided very carefully. The geometry and size of the control volume should be taken according to the geometry of the system and based on the conditions given in the problem. In this case, the geometry of the pipe is cylindrical, hence we use the cylindrical control volume. The fluid is flowing in the z direction but velocity is changing only in r direction. Therefore, the control volume is taken in such a way that the variable thickness of the control volume is in the r direction. As the flow is not dependent on z and θ coordinates, we may choose any dimension in z or θ directions. This means that z may be any length. It may be L/4,

L/2 or L. In a similar manner, any value of θ may be taken. It may be 2 π or $\pi/2$ or $\pi/2$ or $\pi/4$. However, in the r direction, we need to take the differential thickness dr. These arguments leads us to a control volume as shown in Fig. (10.2). The length of the cylindrical shell is L which is equal to length of pipe and thickness is dr.



Fig 10.2 Control volume for flow through pipe Momentum balance As discussed earlier, the shear stress/forces may be written in two ways:

- Taking shear stress as actual shear forces.
- Taking shear stress as momentum flux.

Here, we show that both methods lead to the same final results for velocity profile. Momentum balance using shear stress as shear force Momentum flux entering the control volume by convection

$$\left(\rho v_z^2 2\pi r dr\right)_{z=0}$$

Momentum flux leaving the control volume by convection

$$\left. \left(\rho v_z^2 2 \pi r dr \right) \right|_{z=L}$$

Since the pipe is horizontal, the force due to gravity is zero. No other body forces are acting on the control volume.

Surface forces

• Pressure force: Fluid is flowing in z direction only. So pressure forces which are working on the surface normal to z direction are

Pressure force at z=0 is

$$P_0 2\pi r dr \Big|_{z=0}$$

Pressure force at z=L is

-
$$P_L 2\pi r dr|_{z=L}$$

- Shear forces: The shear stress tensor in cylindrical coordinate is given below.
- $\begin{pmatrix} \boldsymbol{\tau}_{rr} & \boldsymbol{\tau}_{r\theta} & \boldsymbol{\tau}_{rz} \\ \boldsymbol{\tau}_{\theta r} & \boldsymbol{\tau}_{\theta \theta} & \boldsymbol{\tau}_{\theta z} \\ \boldsymbol{\tau}_{zr} & \boldsymbol{\tau}_{z\theta} & \boldsymbol{\tau}_{zz} \end{pmatrix}$

Among all 9 components the first column of stresses are important for r directional flow, the second column of stresses are important for θ directional flow, and the third column are important for z directional flow. Since the fluid is flowing in the z direction, only the third column needs to be considered. Since the Velocity gradient is present only in the r-direction, only τ

 τ_{rz} needs to be considered, the remaining two terms are not significant. Now, we need to decide the direction in which the shear forces are acting. Recall

$$\underline{T}_n = \mathcal{S}_n \cdot \underline{\tau}$$

Where the unit vector \mathcal{Q}_n is the outer normal of a surface and if it is in positive direction then \mathcal{I}_n is also positive while if it is in negative direction then \mathcal{I}_n is shown as negative direction. Therefore, \mathcal{T}_{rz} (as a force) is positive at r+dr and negative at r as shown in Fig. 10.2.(Note: the first index, z, in \mathcal{T}_{rz} from right to left indicates the direction of force and second index, r, indicates the surface on which it acts).

Accumulation term: Due to steady state system, the rate of accumulation of momentum equals to zero .

General momentum balance is given below

$$\begin{pmatrix} rate \ of \ accummulation \\ of \ momentum \ in \ CV \end{pmatrix} = \begin{pmatrix} rate \ of \ momentum \\ entering \ CV \\ by \ convection \end{pmatrix} - \begin{pmatrix} rate \ of \ momentum \\ leaving \ CV \\ by \ convection \end{pmatrix} + (\sum applied \ forces)$$

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or in this case

$$0 = (rv_z^2 2\pi r dr)|_{z=0} - (rv_z^2 2\pi r dr)|_{z=L} + 0 + P_0 2\pi r dr$$
$$- P_L 2\pi r dr + (\tau_{rz} 2\pi r L)|_{r+dr} - (\tau_{rz} 2\pi r L)|_r$$

Since the velocity is constant along the axial direction as shown in Equation (10.2), the first two terms in Equation (10.8) are cancel out and we are left with following Equation.

$$0 = 2\pi L \left[\left(\tau_{rz} r \right) |_{rdr} - \left(\tau_{rz} r \right) |_{rdr} \right] + P_0 2\pi r dr - P_L 2\pi r dr$$

Dividing by $2\pi r dr$, we have

$$0 = \frac{P_0 - P_L}{L} + \frac{(\tau_{rz}r)|_{r+dr} - (\tau_{rz}r)|_r}{rdr}$$

As dr \rightarrow 0, the Equation (10.10) may be rewritten as given below.

(Note that, τ_{rz} is a function of r only which means we get the total derivative instead of the partial derivative.)

$$\frac{d(\tau_{rz}\mathbf{r})}{dr} = \frac{-\mathbf{r}\left(\mathbf{P}_{0} - \mathbf{P}_{L}\right)}{L}$$

Further integrating the Equation (10.11) once with respect to the variable r, we obtain

$$\tau_{rz} \mathbf{r} = -\frac{r^2}{2} \frac{(\mathbf{P}_0 - \mathbf{P}_L)}{L} + C_1$$

or

$$\tau_{\rm rz} = -\frac{r}{2} \frac{({\rm P}_0 - {\rm P}_{\rm L})}{L} + \frac{C_1}{r}$$

Here, c1 is a constant of integration. Equation (10.12) shows that if r=0, the value of τ_{rz} will be infinite, which is physically not possible. Therefore, c1 must be zero. Hence,

$$\tau_{\rm rz} = -\frac{r}{2} \frac{(\rm P_0 - \rm P_L)}{L}$$

Now, by applying Newton's law of viscosity, and taking τ_{rz} as force, we obtain

$$\tau_{\rm rz} = +\mu \, \frac{dv_{\rm z}}{dr} = -\frac{r}{2} \, \frac{({\rm P}_0 - {\rm P}_{\rm L})}{L}$$

Momentum balance using shear stress as momentum flux

Now, we will employ the second method where shear force are considered as momentum flux. To indicate the direction of momentum flux, we draw the arrow in r direction and find where this arrow enters the control volume and also leaves the control volume as shown in Fig (10.3). Thus,

the momentum flux enters the control volume through the surface 2^{π} rL at r=r and leaves through the surface 2^{π} rL at r=r+dr.

Momentum flux <u>heaving</u> Momentum flux Fig 10.3 Momentum flux applied on control volume Thus, Momentum flux at r = r is $(\tau_{rz} 2\pi rL)|_r$ Momentum flux at $r = r + \Delta r$ is $(\tau_{rz} 2\pi rL)|_{r+\Delta r}$

(Note: when we consider τ_{rz} as the momentum flux, first index, z, indicates the direction of momentum flux, while the second index, r, indicates the direction of flow of momentum flux from higher to lower value. Subsequently, it will become clear that if we follow the coordinate system's directions and assume momentum is flowing in this direction, the sign convention for momentum flux is automatically taken place.)

In this case, momentum balance in Equation (9.2) may be modified as shown below

$$\begin{pmatrix} \text{rate of accumulation} \\ \text{of momentum in CV} \end{pmatrix} = \begin{pmatrix} \text{rate of momentum} \\ \text{entering CV} \\ \text{by convection} \end{pmatrix} - \begin{pmatrix} \text{rate of momentum} \\ \text{leaving CV} \\ \text{by convection} \end{pmatrix} + (\sum_{\substack{\text{value} \text{ of viscous} \\ \text{momentum} \\ \text{entering CV} }) - \begin{pmatrix} \text{rate of viscous} \\ \text{momentum} \\ \text{leaving CV} \end{pmatrix}$$

Here, the shear stress are taken into account as momentum flux. The pressure and gravity are the only applied forces.

Substituting various terms in above equation, we obtain

$$0 = 0 + (P_0 - P_L) 2\pi r dr + (\tau_{rz} 2\pi r L) \Big|_r - (\tau_{rz} 2\pi r L) \Big|_{r+dr}$$

.

Dividing by $2\pi r dr$, we obtain

$$0 = (\tau_{rz}r)|_{r} - (\tau_{rz}r)|_{r+dr} + \frac{(P_{0} - P_{L})}{L}$$

Again as dr \rightarrow 0 Equation (10.17) leads to

$$0 = -\frac{d(\tau_{\pi}\mathbf{r})}{rdr} + \frac{(\mathbf{P}_0 - \mathbf{P}_L)}{L}$$

or

$$\frac{d(\tau_{rz}\mathbf{r})}{dr} = \frac{(\mathbf{P}_0 - \mathbf{P}_L)}{L}r$$

By integrating the Equation (10.18), we have

$$\tau_{\rm rz} = \frac{({\rm P}_0 - {\rm P}_{\rm L})}{2L}r + \frac{c_1}{r}$$

As we discussed earlier, c1 should be zero. Therefore,

$$\tau_{\rm rz} = \frac{(\rm P_0 - \rm P_L)}{2L}r$$

Now applying Newton's law of viscosity where shear stress is taken as momentum flux, we obtain

$$\mu \frac{dv_z}{dr} = -\frac{(\mathbf{P}_0 - \mathbf{P}_L)}{2L}r$$

Equation (10.14) and (10.20) are identical and hence show that both methods finally lead to the same result.

To obtain velocity profile we further integrating the Equation (10.21)

$$v_z = -\frac{(P_0 - P_L)}{2\mu L}\frac{r^2}{2} + c_2$$

Here c2 is the second constant of integration which may be determined by using appropriate boundary condition.

Boundary condition

By no-slip boundary condition vz=0 at r=R

$$0 = -\frac{(P_0 - P_L)}{4\mu L}R^2 + c_2$$
$$c_2 = \frac{(P_0 - P_L)}{4\mu L}R^2$$

Substituting the value of c2 in Equation (10.22), we finally get

$$v_{z} = \frac{(P_{0} - P_{L})}{4\mu L} (R^{2} - r^{2})$$

Note: c1 can also be calculated by using the boundary condition in terms of velocity vz: i.e., vz is finite at r=0

$$\left.\frac{dv_z}{dr}\right|_{r=0} = 0$$

or r=0 (since the velocity profile is symmetric about r=0). Thus, the velocity profile for flow through pipe is given by the following expression

$$v_{z} = \frac{(P_{0} - P_{L})}{4\mu L} R^{2} \left(1 - \frac{r^{2}}{R^{2}} \right)$$

The maximum velocity of the fluid will be exhibited at the centre of the pipe and is given by

$$v_{z \max} = v_z |_{r=0} = \frac{(P_0 - P_L)}{4\mu L} R^2$$

Alternatively, the velocity profile may also be expressed in terms of the maximum velocity as

$$v_z = v_{z,\max} \left(1 - \frac{r^2}{R^2} \right)$$

The average velocity of the fluid in the pipe is the average of all local velocities. Thus, this may be calculated by estimating the volumetric flow rate through the pipe and then dividing it by the cross sectional area of the pipe. The total volumetric flow in the system is

$$Q = \int dQ$$

where, dQ is the volumetric flow rate from small cylindrical strip of thickness dr.

$$=\int v_z 2\pi r dr$$

By substituting the value of v z from equation (10.27), we have

$$= \int v_{z max} \left[1 - \frac{r^2}{R^2} \right] 2\pi r dr$$

By integrating the equation (10.30) from r=0 to r=R, we obtain

$$= \int_{0}^{R} 2\pi v_{zmax} \left[r - \frac{r^{3}}{R^{2}} \right] dr$$

or

$$=2\pi v_{zmax} \left[\frac{r^2}{2} - \frac{r^4}{4R^2}\right]_0^R$$

Thus,

$$Q = \pi v_{z \max} \frac{R^2}{2}$$

and average velocity is

$$v_{z,avg} = \frac{Q}{A_c}$$
$$= \frac{\pi v_{z,max}}{\pi R^2}$$

or

$$v_{z,avg} = \frac{v_{z,max}}{2}$$

The velocity profile for laminar flow in a circular tube is shown in Fig. 10.5.



Fig 10.5 Velocity profile in horizontal pipe

We can also find the radial distance at which the local velocity of fluid flow equals the average

velocity. For this, substitute

$$v_z = v_{z,avg} = \frac{v_{z,max}}{2}$$
 into Equation (10.26), we obtain
 $1 - \frac{r^2}{R^2} = \frac{1}{2}$
 $\frac{r^2}{R^2} = \frac{1}{2}$
or, $r = \frac{R}{\sqrt{2}}$

Finally, the volumetric flow rate in terms of pressure drop is as follows

$$Q = v_{zavg} \pi R^2 = \frac{\pi (P_0 - P_L)}{8\mu L} R^4$$
$$Q = \frac{\pi (P_0 - P_L)}{128\mu L} D^4$$

Equation (10.36) is known as the Hagen – Poiseuille equation. Thus, if the pressure drop is given, we can calculate the volumetric flow rate in the pipe and vice-versa. This equation can also be used for the calculation of viscosity in capillary flow viscometer. However, it may be noted that Hagen – Poiseuille equation is valid only for fully developed laminar flow. Therefore, when this equation is used for various calculations there may be some errors due to developing and exiting flow at both ends of the pipe. Hence, this equation has to be modified for real situations.

Friction factor

The friction factor is a dimensionless number, which provides an idea about the magnitude of shear stress produced by a solid boundary as fluid flows. This is defined as the ratio of shear

$$\frac{1}{2}\rho v^2_{zavg}$$

stress at the wall and the kinetic energy head of the fluid,

. Here, ρ is the density

and v_{zavg} is the average velocity of fluid. The friction factor is thereby defined as

$$f = \frac{\tau_w}{\frac{1}{2}\rho v_{zavg}^2}$$

where, τ_w is the shear force per unit area on the wall of the tube. This may be calculated as shown below

$$\tau_w = -\left(-\tau_{rz}\Big|_{r=R}\right)$$

Here, first minus sign is used as the inside surface of the tube wall has outer normal in the negative r direction and second minus sign is used because τ_{rz} is treated here as momentum flux. If τ_{rz} is treated as actual shear force then positive sign would have to be taken. For fully developed laminar flow, the velocity profile is parabolic and is given by

$$v_z = v_{zmax} \left[I - \frac{r^2}{R^2} \right]$$

Evaluating the velocity gradient at the wall (r=R), we have

$$\left.\frac{dv_z}{dr}\right|_{r=R} = -\frac{2v_{z\,max}}{R}$$

Thus, the shear stress considered as momentum flux is given by

$$\tau_{rz}\Big|_{r=R} = -\mu \frac{dv_z}{dr}\Big|_{r=R} = +\frac{2\mu v_{zmax}}{R}$$

or

$$\tau_{w} = \tau_{rz}|_{r=R} = \frac{2\mu v_{zmax}}{R} = \frac{2\mu (P_{0} - P_{L})}{4\mu L} \frac{R^{2}}{R} = \frac{(P_{0} - P_{L})}{2L} R$$

The friction factor may now be calculated as shown below

$$f = \frac{\tau_{w}}{\frac{1}{2}\rho v_{zavg}^{2}} = \frac{\frac{(P_{0} - P_{L})}{2L}R}{\frac{1}{2}\frac{\rho(P_{0} - P_{L})}{8\mu L}R^{2}} = \frac{8\mu}{\rho R v_{zavg}}$$

or

$$f = \frac{16\,\mu}{\rho D v_{zavg}} = \frac{16}{Re}$$

Equation (11.7) shows that the friction factor in laminar flow region depends only on the Reynolds number. Clearly, the friction factor is also a dimensionless number.

Friction factor in turbulent flow



Fig 11.1 Smooth and rough surface of pipe

In turbulent flow, the friction factor also depends on the surface of the pipe. A rough pipe leads to higher turbulence than a smoother pipe, so that the friction factor for smoother pipes is less than

that for rougher pipes. The ratio of surface roughness height (\in) to pipe diameter (D) is used to quantify the "roughness" of the pipe surface. In practice, the shear stress on the wall may be calculated by measuring the pressure drop across the pipe for a given flow rate. Thus, friction factor may be calculated as the function of Reynolds number and plotted on a log-log plot for a given surface roughness. The curves are different for different surface roughness as shown in figure. (11.2). The collection of these f-Re plots is called Moody Chart as shown in figure below, and can be used for estimating the friction factor for given flow parameters.



Ref: http://www.brighthub.com/engineering/civil/articles

Solution of some more fluid flow problems by shell momentum balance approach

In this section, we solve a few more fluid mechanics problems in simple geometries using the shell momentum balance approach. The detail procedure, which was also used in previous example, is outlined below.

1) Make a diagram of the flow geometry with the appropriate coordinate system

- 2) Specify all necessary assumptions
- 3) Intuitively assume the velocity profile

This is an important step for solving these problems. In laminar flow, the fluid flows in parallel layer without mixing. Thus, it is easy to guess the non-zero components of velocities by intuition.

4) Apply of the equation of continuity to modify the velocity profile

5) Determine the non-zero shear stress component(s)

Since the shear stress components depend on the velocity profile, the non-zero shear stress components may now be determine.

6) Determine control volume and make shell momentum balance for the control volume

Draw control volume in system diagram according to system shape, size and problem statement. The selection of proper control volume is very important to solve problem correctly. The control volume should be select in such way that it can be easily integrated for whole system. The differential length of control volume should be taken in direction of changing velocity. Write momentum balance equation for the control volume. The shear stress may be considered as shear force or as momentum flux, both provide the same results as shown in previous example . Write down all surface and body force acting on the fluid carefully. Finally obtain a appropriate differential equation and integrate.

7) Boundary conditions

Use appropriate boundary conditions which help us to determine the constant of integration in above step.

Falling film on an inclined flat surface

An inclined surface of length L and width W is situated at an angle B to the vertical direction as shown in Fig. (11.3). A Newtonian fluid is freely falling on the surface as a film of thickness δ . Assuming the flow to be laminar, determine the velocity profile, flow rate and shear force on the surface by the fluid.

Solution



Fig 11.3 Laminar flow on an inclined surface Assumptions

- Constant density, viscosity
- Steady state
- Laminar flow (simple shear flow)
- Fully developed flow
- Newton's law of viscosity is applicable

Assume velocity profile

The fluid is flowing in the z direction, hence only the z component of velocity is non-zero. Thus, we may assume

$$v_{x} = 0, v_{y} = 0$$

 $v_{z} = v_{z}(x, y, z, t)$ an

We may further assume that vz does not depends upon y coordinate. Since the flow is steady, vz does not depend on time. Thus,

$$v_z = v_z(x, z)$$

Using the equation of continuity in the cartesian coordinates for constant fluid density, we have

$$\frac{\partial v_x}{\partial x} + \frac{\partial v_y}{\partial y} + \frac{\partial v_z}{\partial z} = 0$$

which reduces to

$$\frac{\partial v_z}{\partial z} = 0$$

Equation (11.11) indicates that vz does not depend on the z coordinate. Thus,

 $v_z = v_z(x)$

There are nine components of the shear stress as shear force or momentum flux, namely

 $\tau_{xx} \tau_{xy} \tau_{xz} \rightarrow \text{acting on } x \text{ surface}$ $\tau_{yx} \tau_{yy} \tau_{yz} \rightarrow \text{acting on } y \text{ surface}$ $\tau_{zx} \tau_{zy} \tau_{zz} \rightarrow \text{ acting on } z \text{ surface}$

Since vz is only the non-zero velocity, and also it is the function of x coordinate, t_{zx} is the only significant component of shear stress and we need to write momentum balance only in z direction. Because the pressure is same at both ends of the inclined plane, there is no pressure force on the fluid. Now, we can solve this problem by assuming shear stress as a shear force or shear stress as momentum flux.

Assuming τ_{xz} as momentum flux Draw a control volume of length L, width W and differential thickness dx.



Fig 11.3 Control volume for falling film problem Momentum balance in x direction Rate of momentum flux entering CV due to viscous transport at

$$x = LW\tau_{xz}|_{x}$$

Rate of momentum flux leaving CV due to viscous transport at

$$x + \Delta x = LW\tau_{xz}\Big|_{x+\Delta x}$$

Gravity force acting on fluid in z direction

$$= (LW\Delta x)(\rho g \cos\beta)$$

Rate of momentum flux entering in CV due to convective transport

$$= \left(\left. \rho v_z W dx \, v_z \right) \right|_{z=0}$$

Rate of momentum flux leaving from CV due to convective transport

$$= \left(\rho v_z W dx \, v_z \right) \Big|_{z=L}$$

Now, when above terms are substituted for z-momentum balance, we obtain

$$\left(\rho v_{z} w dv_{z}\right)\Big|_{z=0} - \left(\rho v_{z} w dv_{z}\right)\Big|_{z=L} + LW(\tau_{xz}\Big|_{x} - \tau_{xz}\Big|_{x+\Delta x}) + (LW\Delta x)\left(\rho g\cos\beta\right) = 0$$

Since the velocity vz does not depends on z coordinate, the first two terms cancel out and we obtain

$$LW(\tau_{xz}|_{x} - \tau_{xz}|_{x+\Delta x}) + (LW\Delta x)(\rho g \cos\beta) = 0$$

Dividing Equation (11.19) by volume of the control volume (LW Δx), we have

$$\frac{(\tau_{xz}\mid_{x} - \tau_{xz}\mid_{x+dx})}{\Delta x} + (\rho g \cos\beta) = 0$$

As $\Delta x \rightarrow 0$, The Equation (11.20)simplified to

$$\frac{d\tau_{xz}}{dx} = \rho g \cos \beta$$

The Newton's law of viscosity (here, shear stress is defined as momentum flux) is given by

$$\tau_{xz} = -\mu \frac{dv_z}{dx}$$
$$\frac{d}{dx} \left(-\mu \frac{dv_z}{dx} \right) = \rho g \cos \beta$$

or

$$-\mu \frac{d^2 v_z}{dx^2} = \rho g \cos \beta$$

or

$$\frac{d^2 v_z}{dx^2} = -\left(\frac{\rho g \cos\beta}{\mu}\right)$$

By integrating the Equation (11.25), we have

$$\frac{dv_z}{dx} = -\left(\frac{\rho \, g \cos \beta}{\mu}\right) x + c_1$$

or

$$v_z = -\left(\frac{\rho g \cos\beta}{\mu}\right) \frac{x^2}{2} + c_1 x + c_2$$

The above equation requires two boundary conditions for determining c1 and c2. Boundary conditions

1 At x=0 the liquid surface is in contact with air where the shear stresses at both gas liquid phases should be equal. Thus,

$$\tau_{xz}(air)\Big|_{x=0} = \tau_{xz}(liquid)\Big|_{x=0}$$

Since both may be assumed Newtonian fluids, we have

$$\mu_g \rho_g \frac{dv_{z(air)}}{dx}\Big|_{x=0} = \mu \rho \frac{dv_z}{dx}\Big|_{x=0}$$

where ρg is the density and μg is the viscosity of air. Thus

$$\left. \frac{dv_z}{dx} \right|_{x=0} = \frac{\mu_g \rho_g}{\mu \rho} \frac{dv_{z(air)}}{dx} \right|_{x=0}$$

Since, μg and ρg is much smaller than μ and $\rho,$ and Equation (11.30) may be approximately written as

$$\left.\frac{dv_z}{dx}\right|_{x=0} = 0$$

Substituting above boundary condition in Equation (11.26), we obtain

$$c_1 = 0$$

2. At x= δ no slip boundary condition may be applied, i.e., at

 $x = \delta$ v = 0Thus, from Equation (11.27), we get

$$0 = -\left(\frac{\rho g \cos\beta}{\mu}\right) \frac{\delta^2}{2} x + c_2$$

or

$$c_2 = \left(\frac{\rho g \cos \beta}{\mu}\right) \frac{\delta^2}{2}$$

Finally the velocity profile is obtained as

$$v_z = -\left(\frac{\rho g \cos \beta}{\mu}\right) \frac{x^2}{2} + \left(\frac{\rho g \cos \beta}{\mu}\right) \frac{\delta^2}{2}$$

or

$$v_z = \frac{\rho g \delta^2 \cos \beta}{2\mu} \left(1 - \left(\frac{x}{\delta}\right)^2 \right)$$

Falling film "Assuming $\tau_{\rm XZ}$ as shear force"

Now, we again solve the same problem (falling film over an inclined plane) by treating shear stress as a shear force. For this purpose, we take the same control volume as before. For momentum balance in z direction, all terms are same as before except the terms for shear

forces. Here, τ_{xz} represents the force in z direction acting on the surfaces which have normal in x direction. Shear force is positive if the outward normal is in positive direction and negative if normal is in negative direction. Thus,

shear force at x=x is
$$-LW\tau_{xz}|_{x}$$

Shear force at $x=x+\Delta x$ is + $LW\tau_{xz}|_{x+\Delta x}$;

The z momentum balance for this case is as follows

$$LW(\tau_{xz}|_{x+\Delta x} - \tau_{xz}|_{x}) + (LW\Delta x)(\rho g \cos\beta) = 0$$

Dividing Equation (12.3) by the volume of control volume WL Δx , we have

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

As $\Delta x \rightarrow 0$ Equation (12.4) leads to

$$\frac{d\tau_{xz}}{dx} = -\rho g \cos \beta$$

Now, substituting the Newton's law of viscosity for shear stress as a force

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

Therefore,

$$\mu \frac{d^2 v_z}{dx^2} = -\rho g \cos \beta$$

Equations (11.24) and (12.7) are the same, which show that both approaches provide the same answer.

Maximum velocity

It is clear from Equation (11.37) that the maximum velocity is given by

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

Average velocity and volumetric flow rate of falling film

vz is the linear velocity in z direction. Hence, the volumetric flow rate can be determined by integrating it over the cross section of flow (W δ). Thus,

$$Q = \int_{0}^{W} \int_{0}^{\delta} v_z dx dy$$

From Equation (11.37), we get

$$Q = \int_{0}^{W} \int_{0}^{\delta} \frac{\rho g \delta^2 \cos \beta}{2\mu} \left(I - \left(\frac{x}{\delta}\right)^2 \right) dx dy$$

By integrating Equation (12.10), we find

$$Q = \frac{W \rho g \delta^{\beta} \cos \beta}{3 \mu}$$

To obtain the average velocity, we divide the volumetric flow rate by the cross sectional area.
$$\langle v_z \rangle_{avg} = \frac{Q}{\int\limits_{0}^{W} \int\limits_{0}^{\delta} dx dy}$$

or

$$\langle v_z \rangle_{avg} = \frac{\rho g \delta^2 \cos \beta}{3\mu}$$

Equation (12.12) may also be written as

$$\langle v_z \rangle_{avg} = \frac{2}{3} v_{z,max}$$

Force acting on solid surface due to the fluid

$$F = \int_{0}^{LW} \int_{0}^{W} + \left(+\tau_{xz} \Big|_{x=\delta} \right) dy dz$$

(Note: in Equation (12.14), first '+' sign shows the direction of the normal of the inclined surface and second '+' sign is taken since shear stress is defined as shear force). Thus,

$$F = \rho g \delta L W \cos \beta$$

In this lecture, we have once again seen that the shear stress tensor may be assumed as a shear force or as a momentum flux. In either case, we finally obtain the same expression for the velocity profile. The only difference is that when we treat shear stress as a shear force, it is included in the summation of all forces term in the momentum balance equation, while when we treat shear stress as momentum flux, it is written as momentum entering and leaving by the viscous transport. From now onwards, we will treat shear stress as momentum flux as it is more consistent with what we see in heat transfer as Fourier's law of heat conduction and in mass transfer as Fick's law of diffusion. Thus, in transport phenomena (Momentum transport, Heat transport, and Mass transport) for the basic transport laws we have minus sign in front the relevant gradient implying fluxes flow from higher values to lower values.

Falling film on the outside of a circular shell

In an experiment, a fluid flows upward through a small circular shell and then flows downward out side the tube under laminar conditions as shown in Fig. 12.2. We need to set up a relevant momentum balance and determine the velocity profile, mass flow rate and the force acting on outer surface of the tube.



Fig 12.2 Falling film outside the circular tube Assumptions

- Density and viscosity are constants.
- Steady state.
- Fully developed laminar flow.
- Newton's law of viscosity is applicable.

Non-zero velocities

Fluid is flowing in the z direction due to gravity. There is no driving force in the θ direction and a solid surface is present in the r direction. Therefore, we may intuitively assume that

$$v_z = v_z(r, z)$$
$$v_\theta = 0$$
$$v_r = 0$$

Now, using the equation of continuity in cylindrical coordinate system, we have

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

or

$$\rho \frac{\partial}{\partial z} (v_z) = 0$$

From Equation (12.18), we obtain that vz is independent to z. Therefore,

$$v_z = v_z(r)$$

Choose a control volume in the film of differential thickness dr and length L (it is a cylindrical shell).



 $(\rho v_z 2\pi r \Delta r v_z)|_{z=L}$

Fig 12.3 Control volume for falling film outside the circular tube

There are nine components of shear stress tensor. Since the fluid is flowing in z direction and it is

a function of r only, we may argue as before τ_{rz} is the only important component of the shear stress tensor. The other components are insignificant for momentum balance in z direction. The momentum balance in z-direction is given below.

Momentum balance for control volume Convective momentum entering the control volume at z=0 is

 $(\rho v_z 2\pi r \Delta r v_z)_{z=0}$

Convective momentum leaving the control volume at z=L is

 $(\rho v_z 2\pi r \Delta r v_z)_{z=L}$

Shear stress as momentum flux entering the control volume at r=r is

 $(2\pi r L \tau_{r_2})|_{r=r}$

Shear stress as momentum flux entering the control volume at $r = r + \Delta r$ is

$$(2\pi r L \tau_{rz})_{r=r+\Delta r}$$

.

{Note: If you consider shear stress as momentum flux, then it always flows in the positive direction of axes}

Fluid is flowing only due to gravity and may be written as

 $(2\pi r\Delta rL\rho g)$

Substituting above terms, we obtain

$$(\rho v_{z} 2\pi r D v_{z})|_{z=0} - (\rho v_{z} 2\pi r \Delta v_{z})|_{z=L} + (2\pi r L \tau_{rz})|_{r=r} - (2\pi r L \tau_{rz})|_{r=r+\Delta r} + 2\pi r \Delta r L \rho g = 0$$

Since velocity, vz, is not dependent on the z, the first two terms in above equation are equal and cancel out, leaving the following equation for momentum balance.

$$(2\pi r L \tau_{r_2})\Big|_{r=r} - (2\pi r L \tau_{r_2})\Big|_{r=r+\Delta r} + 2\pi r \Delta r L \rho g = 0$$

Dividing Equation (12.26) by volume of control volume $2\pi r \Delta r L$, we obtain

$$\frac{(r\tau_{rz}|_{r} - r\tau_{rz}|_{r+\Delta r})}{r\Delta r} = -\rho g$$

As dr \rightarrow 0, Equation (12.27) reduces to

$$-\frac{1}{r}\frac{\partial}{\partial r}(r\tau_{rz}) = -\rho g$$

or

$$\frac{1}{r}\frac{\partial}{\partial r}\left(r\left(-\mu\frac{dv_z}{dr}\right)\right) = \rho g$$

After integration we obtain

$$\frac{dv_z}{dr} = -\frac{\rho gr}{2\mu} + \frac{c_1}{r}$$

and

$$v_z = -\frac{\rho g r^2}{4\mu} + c_1 lnr + c_2$$

Here, c_1 and c_2 are the constants of integration. Boundary conditions

1. r=aR we have the air water interface where we may assume that $\frac{d}{dx}$

$$\frac{dv_z}{dr} = 0$$

(The explanation is given earlier in Lecture 11.) Substituting the above boundary condition, we obtain

$$c_1 = \frac{\rho g a^2 R^2}{2\mu}$$

2. At r = R, no slip boundary condition is applicable. Thus,

$$v_z\Big|_{r=R}=0$$

Using this boundary condition, we obtain

$$c_2 = \frac{\rho g R^2}{4\mu} - c_1 \ln R$$

or,

$$c_2 = \frac{\rho g R^2}{4\mu} - \frac{\rho g a^2 R^2}{2\mu} \ln R$$

Therefore, the velocity profile is given by

$$v_{z} = -\frac{\rho g r^{2}}{4\mu} + \frac{\rho g a^{2} R^{2}}{2\mu} lnr + \frac{\rho g a^{2} R^{2}}{4\mu} - \frac{\rho g a^{2} R^{2}}{2\mu} lnR$$

or

$$v_{z} = \frac{\rho g R^{2}}{4 \mu} \left[I - \left(\frac{r}{R}\right)^{2} + 2a^{2} ln\left(\frac{r}{R}\right) \right]$$

Maximum velocity

At r = aR, the velocity is maximum. Thus,

$$v_{z,max} = \frac{\rho g R^2}{4\mu} \Big[1 - \alpha^2 + 2\alpha^2 \ln \alpha \Big]$$

Equation of motion

In this section, we derive the equation of motion, which may be used for solving any fluid mechanics problem. This equation is based on axiom 2, i.e., the momentum is conserved. We consider a control volume having volume $\Delta x, \Delta y, \Delta z$ fixed in space.

According to the momentum conservation equation,

Rate of accumulation of control volume = Net rate of inflow of momentum by convection + net rate of momentum by viscous transport + pressure forces + gravity forces



Fig 15.1 Cubical control volume fixed in space Momentum balance in x direction

Rate of accumulation of x directed momentum in control volume

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

Net rate of inflow of x directed momentum into CV by convection from x-phases

$$\left[(\rho v_{x} \Delta z \Delta y) v_{x}\right]_{x} - \left[(\rho v_{x} \Delta z \Delta y) v_{x}\right]_{x+\Delta x}$$

Net rate of inflow of x-momentum into CV from y-phases

$$= \left[(\rho v_y \Delta x \Delta z) v_x \right]_y - \left[(\rho v_y \Delta x \Delta z) v_x \right]_{y+\Delta y}$$

Net rate of inflow of x-momentum into CV from z-phases

$$= \left[\left(\rho v_z \Delta x \Delta y \right) v_x \right]_z - \left[\left(\rho v_z \Delta x \Delta y \right) v_x \right]_{z+\Delta z}$$

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

In all shear stress component, the second index shows the direction of momentum flux and first

index shows the direction in which the momentum is flowing. For example, τ_{yx} denotes the x directed momentum flowing in y direction. Therefore, the x directed momentum fluxes are

$$\tau_{xx}, \tau_{yx}$$
 and τ_{zx} . Thus,

Net rate of inflow of x directed momentum by viscous transport from x phase are

$$= \left(\tau_{xx} \varDelta z \varDelta y \right) |_{\mathbf{k}} - \left(\tau_{xx} \varDelta z \varDelta y \right) |_{\mathbf{k} + \varDelta x}$$

Net rate of inflow of x directed momentum by viscous transport from y phase are

$$= (\tau_{yx} \Delta x \Delta z)|_{y} - (\tau_{yx} \Delta x \Delta z)|_{y+\Delta y}$$

Net rate of inflow of x directed momentum by viscous transport from z phase are

$$= (\tau_{zx} \Delta x \Delta y) |_{z} - (\tau_{zx} \Delta x \Delta y) |_{z+\Delta z}$$

Net pressure force in x direction =

$$(P \Delta y \Delta z) |_{\mathbf{x}} - (P \Delta y \Delta z) |_{\mathbf{x} + \Delta x}$$

Gravity force in x direction =

$$(\rho \Delta x \Delta y \Delta z) g_x$$

Adding all the above terms and dividing by the volume of control volume $\Delta x, \Delta y, \Delta z$ and finally taking the limits,

 $\Delta x \rightarrow 0$, $\Delta y \rightarrow 0$, and $\Delta z \rightarrow 0$, we obtain

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

The above equation is the x component of equation of motion in cartesian coordinate system. Similarly, for y-direction

$$\frac{\partial(\rho v_y)}{\partial t} = -\left[\frac{\partial(\rho v_x v_y)}{\partial x} + \frac{\partial(\rho v_y v_y)}{\partial y} + \frac{\partial(\rho v_z v_y)}{\partial z}\right] - \left[\frac{\partial \tau_{xy}}{\partial x} + \frac{\partial \tau_{yy}}{\partial y} + \frac{\partial \tau_{zy}}{\partial z}\right] - \frac{\partial \mu}{\partial y}$$

and for z-direction

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

The above three equation may be combined in vector tensor form as

$$\frac{\partial(\rho \mathbf{y})}{\partial t} = -\nabla (\rho \mathbf{y} \mathbf{y}) - \nabla \mathbf{z} - \nabla p + \rho \mathbf{g}$$

In above form, the equation of motion may be used in any coordinate system. Equation (15.14) may be written in substantial derivative form as shown below $\frac{Equation}{\partial t} + \nabla (\rho v v) = -\nabla \tau - \nabla p + \rho g$

if $\stackrel{X}{\sim}$ and $\stackrel{Z}{\sim}$ are the two vectors. We may use the following vector identity.

$$\nabla .(\underline{x}\underline{z}) = \underline{x}.\nabla \underline{z} + \underline{z}(\nabla .\underline{x})$$

Now, replace $\overset{x}{\stackrel{\sim}{}}$ by $\overset{\rho_{\mathcal{V}}}{\stackrel{\sim}{}}$ and $\overset{z}{\stackrel{\sim}{}}$ by $\overset{\nu}{\stackrel{\nu}{}}$, then we have

$$\nabla_{\cdot}(xz) = \nabla_{\cdot}(\rho vv) = \rho v \cdot \nabla v + v (\nabla_{\cdot} \rho v)$$

also,

$$\frac{\partial(\rho v)}{\partial t} = \rho \frac{\partial v}{\partial t} + v \frac{\partial \rho}{\partial t}$$

After substituting Equations, the equation of motion reduces to

$$\underline{v}\frac{\partial\rho}{\partial t} + \rho\frac{\partial v}{\partial t} + \rho \underline{v}.\nabla \underline{v} + \underline{v}(\nabla .\rho \underline{v}) = -\nabla .\underline{\tau} - \nabla p + \rho \underline{g}$$

Rearranging the terms on the left hand side, we have

$$\rho \left[\frac{\partial y}{\partial t} + y \cdot \nabla y \right] + y \left[\frac{\partial \rho}{\partial t} + \nabla \rho y \right] = -\nabla z - \nabla p + \rho g$$

But from the equation of continuity

$$\frac{\partial \rho}{\partial t} + \nabla \cdot \rho y = 0$$

Hence,

$$\rho \left[\frac{\partial \underline{v}}{\partial t} + \underline{v} \cdot \nabla \underline{v}\right] = -\nabla \cdot \underline{\tau} - \nabla p + \rho \underline{g}$$

or

$$\rho \frac{D y}{D t} = -\nabla \cdot z - \nabla p + \rho g$$

Equations (15.20) and (15.21) are the generalized form of equation of motion without any assumption and may be applied to any coordinate system. The detailed form of this equation in cartesian, cylindrical and spherical coordinate system is given in Appendix-3. Navier Stokes Equation for incompressible Newtonian fluid

The equation of motion may be further simplified by substituting the Newton's law of viscosity for the momentum flux term appearing in the equation of motion. For a one-dimensional system where

vy=0,vz=0

we have seen that the Newton's law of viscosity may be written as,

$$\tau_{yx} = -\mu \frac{\partial v_x}{\partial y}$$

where, τ_{yx} represents x directed momentum flowing in the y direction However, in general, for a three dimensional flow, all 9 components of shear stress may be important. Thus,

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

Here, τ_{xx} , τ_{yy} and τ_{zz} are the normal stresses and the remaining are shear stress. Axiom 3: Moment of momentum is conserved

This axiom 3 leads to a very simple conclusion that the shear stress tensor is symmetric in nature. The derivative itself is lengthy and is not reproduced here. \mathcal{I} is symmetric implies that

$$\tau_{xy} = \tau_{yx}$$
$$\tau_{xz} = \tau_{zx}$$
$$\tau_{yz} = \tau_{zy}$$

Newton's law of viscosity may now be generalized as given below. Again, the basis for this representation is not shown here, but it may be found in any standard books in fluid mechanics.

$$\underline{\tau} = -\mu \underline{\Delta} + \frac{2}{3} \mu(\nabla \underline{v}) \delta_{ij} \underline{\delta}_i \underline{\delta}_j$$

where,

$$\underline{\mathcal{A}} = \left(\frac{\partial v_i}{\partial x_j} + \frac{\partial v_j}{\partial x_i}\right) \underline{\mathcal{S}}_i \underline{\mathcal{S}}_j$$

Hence, we have the nine components of shear stress as

$$\tau_{xx} = -2\mu \frac{\partial v_x}{\partial x} + \frac{2}{3}\mu \nabla v_x$$

$$\tau_{yy} = -2\mu \frac{\partial v_y}{\partial y} + \frac{2}{3}\mu \nabla v_x$$

$$\tau_{zz} = -2\mu \frac{\partial v_z}{\partial z} + \frac{2}{3}\mu \nabla v_x$$

$$\tau_{xy} = \tau_{yx} = -\mu \left(\frac{\partial v_x}{\partial y} + \frac{\partial v_y}{\partial x}\right)$$

$$\tau_{yz} = \tau_{zy} = -\mu \left(\frac{\partial v_z}{\partial y} + \frac{\partial v_y}{\partial z}\right)$$

$$\tau_{xz} = \tau_{zx} = -\mu \left(\frac{\partial v_z}{\partial z} + \frac{\partial v_z}{\partial z}\right)$$

The detail form of Newtons law of viscosity in all coordinate system is given in Appendix- 01. Now, consider the situation when an incompressible fluid is flowing only in x direction and

depends on y coordinate only. In such a case, we have $v_x = v_x(y)$, $v_y = 0$ and $v_z = 0$. We can easily see that for this case,

$$\tau_{xx} = \tau_{yy} = \tau_{zz} = 0$$

$$\tau_{yz} = \tau_{zy} = 0$$

$$\tau_{xz} = \tau_{zx} = 0$$

and only significant components of stress are τ_{xy} and τ_{yx} . Also, the expression for the same as given earlier as Newton's law of viscosity. For rectangular coordinate system, substituting the value of $-\nabla \tau$ in the x component of equation of motion, we obtain

$$-\left(\nabla_{x} \cdot \tau\right)_{x} = -\left[\frac{\partial \tau_{xx}}{\partial x} + \frac{\partial \tau_{yx}}{\partial y} + \frac{\partial \tau_{zx}}{\partial z}\right]$$

Assuming that ρ and μ are constant, we obtain

$$-\nabla \underline{\tau} = -\left[\frac{\partial}{\partial x}\left(-2\mu\frac{\partial v_x}{\partial x}\right) + \frac{\partial}{\partial y}\left(-\mu\left(\frac{\partial v_x}{\partial y} + \frac{\partial v_y}{\partial x}\right)\right) + \frac{\partial}{\partial z}\left(-\mu\left(\frac{\partial v_z}{\partial x} + \frac{\partial v_x}{\partial z}\right)\right)\right]$$

or

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

or

$$= \mu \left[\frac{\partial^2 v_x}{\partial x^2} + \frac{\partial^2 v_x}{\partial y^2} + \frac{\partial^2 v_x}{\partial z^2} + \frac{\partial}{\partial x} \left[\frac{\partial v_x}{\partial x} + \frac{\partial v_y}{\partial y} + \frac{\partial v_z}{\partial z} \right] \right]$$

But from equation of continuity for an incompressible fluid, we have

$$\frac{\partial v_x}{\partial x} + \frac{\partial v_y}{\partial y} + \frac{\partial v_z}{\partial z} = 0$$

Therefore,

$$-\left(\nabla_{x}\cdot\overline{z}\right)_{x} = \mu \left[\frac{\partial^{2}v_{x}}{\partial x^{2}} + \frac{\partial^{2}v_{x}}{\partial y^{2}} + \frac{\partial^{2}v_{x}}{\partial z^{2}}\right]$$
$$= \mu \left[\frac{\partial^{2}}{\partial x^{2}} + \frac{\partial^{2}}{\partial y^{2}} + \frac{\partial^{2}}{\partial z^{2}}\right]v_{x}$$

or

$$-\left(\nabla_{x} \cdot \tau\right)_{x} = \mu \nabla^{2} v_{x}$$

 $- \left(\nabla . \tau \right)_y = \mu \nabla^2 v_y$

similarly

$$-\left(\nabla_z \cdot \tau\right)_z = \mu \nabla_z^2 v_z$$

Therefore, in vector and tensor form

$$-\left(\nabla \cdot \underline{\tau}\right) = \mu \nabla^2 \underline{v}$$

Thus, the equation of motion reduce to

$$\rho \frac{Dv}{Dt} = -\nabla p + \mu \nabla^2 v + \rho g$$

Equation (16.25) is known as the Navier Stokes equation and is used for solving problems involving Newtonian fluids of constant density and viscosity. For non-Newtonian and compressible fluids, the generalized form of equation of motion given earlier must be used. Solution of momentum transport problems using Navier Stokes equation In this section, transport problems involving Newtonian fluids are solved by making use of the equation of motion or Navier Stokes equation. We will firstly solve the falling film problem and flow through a circular tube for comparing the solutions obtained earlier by using the momentum balance



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Falling film on an inclined surface



Fig 17.1 Falling film on inclined surface

This problem was solved earlier by the shell momentum balance technique. We will now try to solve this problem by using the Navier Stokes equations.

We are again required to make the same necessary assumptions as done earlier using the shell momentum balance technique. We postulate the non- zero components of the velocity and from there, determine the non-zero components of the shear stress tensor. These steps are the same as

earlier and lead us to conclude that $v_z = v_z(r)$ and τ_{rz} is the only important component of shear stress. We now use the Navier Stokes equation in cartesian coordinates as given in Appendix-03.

$$\rho g_r = 0$$

x component is

y component is

$$\rho g_y = 0$$

z component is

$$\mu \frac{d^2 v_z}{dx^2} + \rho g_z = 0$$

where

$$g_z = g \cos\beta$$

Integrating Equation (17.3), we have

$$\frac{dv_z}{dx} = -(g\cos\beta)x + c_1$$

and

$$v_z = -(g\cos\beta)x + c_1x + c_2$$

The boundary conditions are also the same as used earlier, at

$$x = 0, \left. \frac{dv_z}{dx} \right|_{x=0} = 0$$

and at

This leads to the solution for velocity profile, as

$$v_{z} = -\frac{g\delta^{2}\cos\beta}{2\mu} \left[1 - \left(\frac{x}{\delta}\right)^{2} \right]$$

which is same as obtain earlier using shell momentum balance approach.

Fluid flow through a vertical tube

A Newtonian fluid is flowing inside a vertical tube having circular cross section due to pressure difference and gravity. Solve the problem using the Navier Stokes equations.



Fig 17.2 Flow through a vertical circular tube

A similar type of problem (for a horizontal pipe) was solved earlier using the shell momentum balance technique. Therefore, the initial steps are the same and include making appropriate assumptions and postulating the non- zero velocity components. As shown earlier, it leads to the

$$v_z = v_z (r$$

conclusion that

Now using the Navier Stokes equation for cylindrical co-ordinates, after eliminating all zero terms, we have r- component of Navier Stokes equation

$$\frac{\partial P}{\partial r} = 0$$

 θ -component

$$\frac{\partial P}{\partial \theta} = 0$$

z - component

$$\frac{\partial P}{\partial z} + \mu \frac{1}{r} \frac{\partial}{\partial r} \left(r \frac{\partial v_z}{\partial r} \right) + \rho g_z = 0$$

We can combine gravity and pressure forces as to rewrite Equation (17.11) as,

$$-\frac{\partial P_c}{\partial z} + \mu \frac{1}{r} \frac{\partial}{\partial r} \left(r \frac{\partial v_z}{\partial r} \right) = 0$$

where, Pc is the effective pressure including the gravity, and is defined as,

$$P_c = P - \rho g_z Z$$

Note that since pressure changes in only z direction and vz is a function of r only the partial derivative may be converted to total derivative. Furthermore, in Equation (17.12), the first term is only a function of z and the second term is only a function of r, i.e.,

$$F_I(z) + F_2(r) = 0$$

This leads to result that F1 and F2 both are constants as Equation (17.13) is true for all values of z and r.

$$F_{I}(z) = c_{I}; F_{2}(r) = -c_{I}$$

Therefore,

$$\frac{dP_c}{dz} = c_1$$

By integrating the Equation (17.15)

$$P_c = c_1 z + c_2$$

Boundary conditions are at

$$\inf_{and} = 0, P_c = P_{c0}$$

This leads to the following solution

$$z = L, P_c = P_{cL}$$

$$\frac{P_{c0} - P_{cL}}{L} = c_1$$

By substituting in Equation (17.12)

$$-\left(\frac{P_{c0} - P_{cL}}{L}\right) + \mu \frac{l}{r} \frac{d}{dr} \left(r \frac{dv_z}{dr}\right) = 0$$

or

$$v_z = -\left(\frac{P_{c0} - P_{cL}}{4\mu L}\right)r^2 + c_3\ln r + c_4$$

Boundary conditions are at r=0, v z is finite and

at
$$r = R$$
,
 $v_z = 0$

This leads to

$$v_{z} = \left(\frac{P_{c0} - P_{cL}}{4\mu L}\right) R^{2} \left[I - \left(\frac{r}{R}\right)^{2} \right]$$

which is again similar to what we have seen for a horizontal tube except for pressure difference term. In fact, it can be shown that the velocity profile given in Equation (17.22) is valid for any configuration, horizontal, vertical, or inclined, with effective pressure is defined as

$$\begin{split} P_{c} &= P - \rho g_{z} z \\ T_{z} &= \int_{0}^{2\pi} \int_{0}^{R} (-\tau_{\text{GF}}) |_{\theta=\pi/2} r dr r d\phi = 2\pi \left(\frac{\mu \Omega}{\psi}\right)_{0}^{R} r^{2} dr \end{split}$$

$$v_{\theta} = v_{\theta}(r, z)$$

For simplifying the problem further, we may assume that for low shear rates

$$\mathbf{v}_{\theta} = rf(z)$$

Using the θ component of the Navier – Stokes equation for cylindrical co-ordinate systems

$$\frac{\partial}{\partial r} \left(\frac{1}{r} \frac{\partial}{\partial r} (r v_{\theta}) \right) + \frac{\partial^2 v_{\theta}}{\partial z^2} = 0$$

By substituting Equation (19.25), we get

$$\frac{\partial}{\partial r} \left(\frac{1}{r} \frac{\partial}{\partial r} \left(r^2 f(z) \right) \right) + \frac{r \partial^2 f(z)}{\partial z^2} = 0$$

or
$$\frac{\partial^2 f(z)}{\partial z^2} = 0$$

$$f(z) = c_1 z + c_2$$

After integration, we finally obtain

where C_{1} and C_{2} are the integral constant.

Boundary conditions are

at
$$z = 0$$
, $v_{\theta} = 0$ or $f(z) = 0$

thus,

$$c_2 = 0$$

and at z = B, $v_{\theta} = v_{\text{or}}$ $f(z) = v/r = \Omega$ $r \partial \theta$

Now, the *z*-component of the torque exerted on the fluid by the upper rotating disc, may be calculated as

$$T_{z} = \int_{0}^{2\pi} \int_{0}^{R} (-\tau_{z\theta}) r |_{z=B} r dr d\theta$$

or

$$= 2\pi\mu \frac{\Omega}{r} \int_{r}^{R} r^{3} dr$$
$$T_{z} = \pi\mu \frac{\Omega}{2B} R^{2}$$

Thus, by plotting the angular velocity Ω vs torque T_z , the viscosity may be

Non-Newtonian fluids

Non-Newtonian fluids are the fluids which do not obey Newton's law of viscosity. For describing Non-Newtonian fluids, let's recall the Newton's law of viscosity experiment. There are two long parallel plate situated at distance h to each other. Top plate is stationary and bottom

plate is moving with velocity $\frac{y}{2}$ as shown in Fig. (20.1).



Fig 20.1 Non-Newtonian flow between two parallel plates

If a force, F, is applied to move plate, then (τ_{xy}) $\tau_{xy} = \frac{F}{A}$

and under steady state conditions when h is small and when

$$\frac{dv_x}{dy} = \frac{v}{h}$$

Now, we calculate τ_{xy} by repeating experiments for different applied forces and velocity achieved by the bottom plate and plotting a graph as shown in Fig. (20.2). Depending on the nature of fluid, different types of curves may be obtained.





Rheological behaviour of fluids

If fluid shows the behaviour like curve (1) then it is a Newtonian fluid. Other fluids are non-Newtonian fluids. Curve (2) represents a Pseudo-plastic fluid, curve (3) represents a Dilatant fluid, and curve (4) represents a Bingham plastic fluid. There are several Theoretical and empirical models available to describe the rheological behaviour of non-Newtonian fluids. Here, we discuss some of them, which come under the group of generalized Newtonian models. Basic equation for a generalized non-Newtonian fluid is given below

$$\tau_{yx} = -\eta \, \frac{dv_x}{dv}$$

Here, η is the apparent viscosity, which is clearly a function of shear rate as may be seen. Therefore,

 $\eta = f\left(\frac{dv_x}{dy}\right)$

If the apparent viscosity increases with increase in shear rate, dy

Dilatant fluid and if it decreases with increase in shear rate, dy then fluid is called Pseudoplastic fluid. Some fluids require a critical shear stress to initiate the flow. These fluids are called Bingham fluids. Some important rheological models for non-Newtonian fluids are given below.

 dv_x

, then the fluid is called

1 Power Law or Ostwald De Waele model

Power law or Ostwald De Waele model is the most generalized model for non-Newtonian fluids. The expression of this model is given in Equation (20.3)

$$\tau_{yx} = -m \left| \left(\frac{dv_x}{dy} \right) \right|^{n-1} \frac{dv_x}{dy}$$

Here, apparent viscosity η is defined as,

$$\eta = m \left| \left(\frac{dv_x}{dy} \right) \right|^{n-1}$$

This is a two-parameter model where m and n are the two parameters.

If n = l then $\eta = m$

where m is similar to the viscosity of the fluid and model shows the Newtonian behaviour .

If n>1, then η increases with increasing shear rate and the model shows the Dilatant behaviour.

If n<1, then η decreases with increasing shear rate and the model shows the Pseudo-plastic behaviour.

Modulus sign

In power law model, modulus sign can be removed according to the value of shear rate.

1. If
$$\frac{dv_x}{dy}$$
 is positive, then

$$\eta = m \left(\frac{dv_x}{dy}\right)^{n-1}$$

2. If
$$\frac{dv_x}{dy}$$
 is negative, then

$$\eta = m \left(-\frac{dv_x}{dy} \right)^{n-1}$$

Several fluids do not show single type of rheological behaviour. They show Newtonian behaviour for a range of shear stress and Non-Newtonian behaviour for some other ranges of shear stresses. Several models have been suggested for these types of fluids. Some popular models like Eyring model, Ellis model, Reiner Philipp off model and Bingham Fluid model are discussed here.

2. Eyring model

Eyring model is a two-parameter model. The equation of Eyring model is as follow

$$sinh\left(\frac{\tau_{yx}}{A}\right) = -\frac{1}{B}\frac{dv_x}{dy}$$

where A, B are the two parameters.

In Eyring model, if $\tau_{xy} \rightarrow 0$ which means very low shear forces, we have

$$sinh\left\{\frac{\tau_{yx}}{A}\right\} \rightarrow \frac{\tau_{yx}}{A}$$

Therefore, as $\tau_{yx} \rightarrow 0$, the model shows Newtonian behaviour

$$\tau_{yx} = -\frac{A}{B}\frac{dv_x}{dy}$$

Here, viscosity = $\left(\frac{A}{B}\right)$

If τ_{yx} is very large, the model shows Non-Newtonian behaviour as shown Fig. 20.3



Fig 20.3 Shear stress vs. shear strain diagram for Eyring model

Therefore, Eyring model may be used for a fluid which shows Newtonian behaviour at low shear rates and non- Newtonian behaviour at high shear rates.

3. Ellis model

Ellis model is a three-parameter model. The equation of this model is as follows

$$-\frac{dv_x}{dy} = \left\{ \varphi_o + \varphi_i \left| \tau_{yx} \right|^{\alpha - l} \right\} \tau_{yx}$$

Here, φ_0 , φ_1 and α are the three parameters. Here, we consider some special cases,

1. If
$$\varphi_1 = 0$$
 then Equation (20.11) reduce to

$$\frac{dv_x}{dy} = -\varphi_0 \tau_{yx}$$

or

$$\tau_{yx} = -\frac{1}{\varphi_0} \frac{dv_x}{dy}$$

which is same as Newton's law of viscosity with φ_0 as the viscosity of the fluid.

1

2. If
$$\varphi_0 = 0$$
, then
$$-\frac{dx}{dy} = -\varphi_1 |\tau_{yx}|^{a-1} \tau_{yx}$$

which is similar to a Power law model

3. If $\alpha > 1$ and τ_{yx} is small then the second term is approximately zero and equation reduces to

$$\tau_{yx} = -\frac{l}{\varphi_0} \frac{dv_x}{dy}$$

which is similar to Newton's law of viscosity.

4. If α <1 and τ_{yx} is very large, then again, second term is negligible and we have

$$\tau_{yx} = -\frac{l}{\varphi_0} \frac{dv_x}{dy}$$

Which again shows Newtonian behaviour. Therefore, Ellis model may be used for fluids which show Newtonian behaviour at very low and very high shear stresses, but non-Newtonian behaviour at intermediate value of shear stresses.



Fig 20.4 Shear stress vs. shear strain diagram for Ellis model This type of behaviour may be shown by some polymer melts 4. Reiner Philipp off model

This is also a three-parameter model. The equation of Reiner Philipp off model is as follows,

$$-\frac{dv_x}{dy} = \begin{bmatrix} \frac{1}{\mu_{\infty} + \frac{\mu_0 - \mu_{\infty}}{1 + \left(\frac{\tau_{yx}}{\tau_z}\right)^2}} \end{bmatrix} \tau_{yx}$$

where, μ_0 , μ_∞ and τ_s are the three parameters.

In Reiner Philipp off model, if τ_{yx} is very large, the equation reduces to,

$$-\frac{dv_x}{dy} = \frac{1}{\mu_{\infty}}\tau_{yx}$$

or

$$\tau_{yx} = -\mu_{\infty} \, \frac{dv_x}{dy}$$

which is same as the Newton's law of viscosity,

If τ_{yx} is very small then equation reduces to

$$-\frac{dv_x}{dy} = \frac{1}{\mu_0}\tau_{yx}$$

or

$$\tau_{yx} = -\mu_0 \frac{dv_x}{dy}$$

which is also same as the Newton's law of viscosity. Therefore, Reiner Philipp off model may be used for a fluid which shows Newtonian behaviour at very low and very high shear stresses but non-Newtonian behaviour for intermediate values of shear stress. Here, μ_0 and μ_0 represent the viscosity of fluid at very low and very high shear stress conditions respectively.

5. Bingham Fluid model

Bingham fluid is special type of fluid which require a critical shear stress to start the flow. The equation of Bingham fluid model are given below

$$\tau_{yx} = -\left[\mu + \frac{\tau_0}{\left|\frac{dv_x}{dy}\right|}\right] \frac{dv_x}{dy}$$
if

$$\mid \tau_{_{yx}} \mid > \tau_{_0}$$



$$\frac{d\mathbf{k}}{d\mathbf{y}} = 0$$

A typical shear stress vs. shear rate diagram for a Binghum model is shown below



Fig 20.5 Shear stress vs. shear strain diagram for Bingham model Momentum transport problems involving Power law and Bingham fluids:

In this section, we will solve fluid mechanics problem for Power law and Bingham plastic fluids. These problems have been earlier solved for Newtonian fluids. We have chosen the same problems here for better understanding.

Falling film on inclined plane



Fig 21.1 Falling film problem for non-Newtonian fluid

Initial steps, such as making appropriate assumptions, finding important velocity components, applying equation of continuity, and determining important shear stress components are similar as steps seen for Newtonian fluid in lecture 11 and 17. As before $v_z = v_z(x)$ and is the only non-zero velocity component and τ_{xz} is the only important shear stress component. (Note: Since the forms of shear stress $\tilde{\tau}$ for Newtonian and non-Newtonian fluids are same, the only difference is the viscosity μ for Newtonian fluids and apparent viscosity η for non-Newtonian fluids and furthermore as non-zero components of velocities are also same, the same components of shear stress $\tilde{\tau}$ are significant for both Newtonian and non-Newtonian fluids.) To solve the problem, we start with the generalized equation of motion in terms of $\tilde{\tau}$. Since the fluid is moving in z direction, discarding all terms which are zero, z-component of the equation of motion reduces to

$$-\frac{d\tau_{xz}}{dx} + \rho g_z = 0$$

where

$$g_z = g \cos \beta$$

therefore,

$$\tau_{xz} = \rho g \cos \beta x + c_1$$

For Power law fluids

 $\tau_{xz} = -\eta \frac{dv_z}{dx}$ $\eta = m \left| \frac{dv_z}{dx} \right|^{n-1}$

Since vz is decreasing with increasing value of \boldsymbol{x} , the negative sign should be used for removing the modulus sign, i.e. ,

$$\tau_{xz} = -m \left(-\frac{dv_z}{dx} \right)^{n-1} \left(\frac{dv_z}{dx} \right)$$

or

$$\tau_{xz} = m \left(-\frac{dv_z}{dx} \right)^n$$

By substituting in above,

$$\left(-\frac{dv_z}{dx}\right)^n = \frac{\rho g \cos \beta}{m} x + c_1$$

$$x = 0, \quad \tau_{xz}\big|_{air} = \tau_{xz}\big|_{fluid}$$

By applying the boundary condition, at which simplifies to

$$\left.\frac{dv_z}{dx}\right|_{x=0} = 0$$

as disused in lecture 11

By substituting this boundary condition in Equation (21.8), we get

 $c_1 = 0$. Therefore,

$$\left(-\frac{dv_z}{dx}\right)^n = \frac{\rho g \cos\beta}{m} x$$

or

$$v_z = -\sqrt[n]{\frac{\rho g \cos \beta}{m}} \frac{x^{\frac{l}{n+l}}}{\frac{l}{n}+l} + c_2$$

Here, C_2 is another integral constant.

Now, using the second boundary condition, at $x = \delta$, $v_z = 0$, we finally obtain

$$v_{z} = \frac{n}{n+1} \sqrt[n]{\frac{\rho g \cos \beta}{m}} \delta^{\frac{n+1}{n}} \left[1 - \left(\frac{x}{\delta}\right)^{\frac{n+1}{n}} \right]$$

Tube flow problem for Power law fluid


Fig 21.1 Flow through pipe for non-Newtonian fluid

As we discussed in lecture 10, the only non-zero component of velocity is vz, which depends on r only. The important component of shear stress is τ_{rz} .

By applying general equation of motion in cylindrical co-ordinate, we get

$$\frac{\partial P}{\partial z} - \frac{1}{r} \frac{\partial}{\partial r} (r\tau_{rz}) = 0$$

Equation (21.11) may be further simplified as before

$$\frac{P_0 - P_L}{L} - \frac{1}{r} \frac{\partial}{\partial r} (r\tau_{rz}) = 0$$

or

$$\tau_{rz} = \frac{(P_0 - P_L)}{2L}r + \frac{c_1}{r}$$

By applying the boundary condition, at r=0, velocity is finite, we obtain

$$c_{1} = 0$$

and for power law fluids

$$\tau_{rz} = m \left(-\frac{dv_z}{dr} \right)^n$$

(Note: Since vz is decreasing with increasing value of r, the negative sign should be used for removing the modulus sign.)

By substituting Equation (21.13) to Equation (21.12), we get

$$m\left(-\frac{dv_z}{dr}\right)^n = \frac{(P_0 - P_L)}{2L}r$$

Integrating above equation, we obtain

$$v_{z} = -n \sqrt{\frac{(P_{0} - P_{L})}{2Lm}} \frac{r^{\frac{n+l}{n}}}{\frac{n+l}{n}} + c_{2}$$

Now, by applying the no-slip boundary condition at,

$$c_2 = -n \sqrt{\frac{(P_0 - P_L)}{2Lm}} \frac{R^{\frac{n+1}{n}}}{\frac{n+1}{n}}$$

Thus,

$$v_{z} = \sqrt[n]{\frac{(P_{0} - P_{L})}{2Lm}} \frac{\frac{R^{\frac{n+l}{n}}}{n+l}}{\frac{n+l}{n}} \left[1 - \left(\frac{r}{R}\right)^{\frac{n+l}{n}} \right]$$

Equation (21.15) represents the velocity profile of freely falling film on an inclined surface for a Power law non-Newtonian fluid. If we substitute the n=1 and m= μ in this expression, we get Equation (10.25) which was derived earlier for a Newtonian fluid. Tube Flow Problem for a Bingham Fluid

$$r = R, v_z = 0$$



Fig 22.1 Flow through pipe for Bingham fluid

As mentioned in the previous lecture, the forms of shear stress z for Newtonian and non-Newtonian fluids are the same. Therefore, Equation (21.12) is applicable for a Bingham fluids also, i.e.,

$$\tau_{rz} = \frac{(P_0 - P_L)}{2L}r$$

Equations (20.19) and (20.20) may be written for this system

- 1. For $\tau_{rz} < \tau_0$ ($r < r_0$), where r_0 is to be determine latter, $\frac{dv_z}{dr} = 0$, or $v_z = v_0$ (constant)
- 2 For $\tau_{rz} \ge \tau_0 r \ge r_0$

$$\eta = \mu_0 + \frac{\tau_0}{\left|\frac{dv_z}{dr}\right|}$$

$$\frac{dv_z}{dv_z}$$

In Equation (22.2), dr is negative. Therefore, after removing the modulus sign, we obtain

$$\eta = \mu_0 - \frac{\tau_0}{\left(\frac{dv_z}{dr}\right)}$$

Thus,

$$\tau_{rz} = -\left\{\mu - \frac{\tau_0}{\frac{dv_z}{dr}}\right\} \frac{dv_z}{dr}$$

or

$$\tau_{rz} = -\mu \frac{dv_z}{dr} + \tau_0$$

Condition for movement of fluid

As we start to pressurize the fluid by imposing pressure difference, fluid does not move initially. As we continue to increase the pressure difference the fluid may start to move at some critical

pressure difference ($P_{c0} - P_{cL}$). This critical value may be determined by setting $\tau_{rz}\Big|_{r=R} = \tau_0$ Thus

$$\tau_0 = \frac{\left(P_{c0} - P_{cL}\right)}{2L} R$$

Thus, the fluid will flow if

$$\tau_0 \leq \frac{(P_{c0} - P_{cL})}{2L} R$$

Suppose the pressure difference across the tube exceeds this critical value of pressure (

 $P_{c0} - P_{cL}$ then the fluid will start to flow. Now, under this condition we may calculate the value of (r0) where the value of $\tau_{rz} = \tau_0$. For r<r0, the velocity gradient is zero and the

fluid flows with a constant velocity. The detail calculation for two different regions r < r0 and r > r0 are given below.

$$\tau_{rz} = \frac{(P_0 - P_L)}{2L}r$$
At
$$r = r_0, \tau_{rz} = \tau_0$$
. Thus,
$$\tau_0 = \frac{(P_0 - P_L)}{2L}r_0$$

or

$$r_0 = \frac{2\tau_0 L}{(P_0 - P_L)}$$

For r<r0, we equate Equations (21.12) and (22.4), that is

$$-\mu \frac{dv_{z}}{dr} + \tau_{0} = \tau_{z} = \frac{(P_{0} - P_{L})}{2L}r$$

Finally, we obtain,

$$v_z = \frac{\tau_0}{\mu} r - \left(\frac{(P_0 - P_L)}{4\mu L}r^2\right) + c_I$$

No slip Boundary condition at r=R, $v_z = 0$ may be used to calculate c1 as shown below Substituting this value in Equation (22.11), we get

$$c_{l} = \left(\frac{(P_{0} - P_{L})}{4\mu L}R^{2}\right) - \frac{\tau_{0}}{\mu}R$$

Finally, the velocity profile is given by

$$v_z = \frac{\tau_0}{\mu} (r - R) + \left(\frac{(P_0 - P_L)}{4\mu L} R^2\right) \left(1 - \left(\frac{r}{R}\right)^2\right)$$

Equation (22.12) gives the velocity profile is region $r_0 \le r \le R$, as shown in Fig. 22.2. Equation (22.9) shows that as we keep increasing the pressure difference $(P_0 - P_L)$, the value of r0 keep on decreasing and the velocity profile changes as shown in Fig. 22.2. The value of r0 also depends on τ_0 , and reduces with it. If we substitute $\tau_0 = 0$ in Equation (22.12), we obtain the same expression for velocity profile as we had earlier obtain for

Newtonian fluids. This result implies that if the value of pressure difference $(P_0 - P_L)$ is significantly high then the Bingham fluid may show behaviour similar to Newtonian fluids.



Fig 22.2 Effect of differential pressure flow through pipe for Bingham fluid Now, we may determine the velocity profile in the plug flow region (r>r0) by substituting r=r0 in Equation (22.12)

$$v_0 = \frac{\tau_0}{\mu} (r_0 - R) + \left(\frac{(P_0 - P_L)}{4\mu L} R^2\right) \left(I - \left(\frac{r_0}{R}\right)^2\right)$$

Falling film problem for Bingham fluid

$$\eta = \mu_0 \pm \frac{\tau_0}{\left|\frac{dv_z}{dx}\right|}$$

$$\frac{dv_z}{dx} = 0$$

$$v_z = v_0$$

For region (2) where $\tau \ge \tau_0$ and $\delta \ge \delta_0$, we have



$$dv_z$$

Here dx is negative. Therefore, after removing the modulus sign and substituting the value of η in Generalized Newton's law of viscosity. we obtain,

$$v_{0} = \frac{\rho g \cos \beta \delta^{2}}{2\mu} \left[1 - \frac{\delta_{0}^{2}}{\delta^{2}} \right] - \frac{\tau_{0} \delta}{\mu} \left[1 - \frac{\delta_{0}}{\delta} \right]$$
$$\tau_{xz} = -\left\{ \mu \frac{dv_{z}}{dx} - \tau_{0} \right\} = \rho g \cos \beta x$$

or

 $-\mu \frac{dv_z}{dx} = \rho g \cos \beta x - \tau_0$

$$\frac{dv_z}{dx} = \frac{-\rho g \cos \beta x}{\mu} + \frac{\tau_0}{\mu}$$

Finally, we obtain the velocity profile, as given below

$$v_z = \frac{-\rho g \cos \beta x^2}{\mu} + \frac{\tau_0}{2} + \frac{\tau_0}{\mu} x + c_2$$

where c2 is an integral constant. By using no slip boundary condition at $x = \delta$, $v_z = 0$, we obtain

$$c_2 = \frac{\rho g \cos \beta}{\mu} \frac{\delta^2}{2} - \frac{\tau_0}{\mu} \delta$$

Therefore,

$$v_{z} = \frac{\rho g \cos \beta \delta^{2}}{2\mu} \left[1 - \frac{x^{2}}{\delta^{2}} \right] - \frac{\tau_{0} \delta}{\mu} \left[1 - \frac{x}{\delta} \right]$$

Equation shows the velocity profile in region $\delta_0 \le x \le \delta$. calculate the velocity of plug flow region by substituting the value $x = \delta_0$

EQUATION OF MOTION

Depending on how the fluid and the solid boundaries contact each other, the flow may be classified as internal flow or external flow. In internal flows, the fluid moves between solid boundaries as is the case when fluid flows in a pipe or a duct. In external flows, however, the fluid is flowing over an external solid surface, the example may be sited is the flow of fluid over a sphere as shown in Fig. 8.1.

or



Fig External flow around a sphere Boundary layers and fully developed regions Let us now consider the example of fluid flowing over a horizontal flat plate as shown in Fig.

The velocity of the fluid is before it encounters the plate. As the fluid touches the plate, the velocity of the fluid layer just adjacent to the plate surface becomes zero due to the no slip boundary condition. This layer of fluid tries to drag the next fluid layer above it and reduces its velocity. As the fluid proceeds along the length of the plate (in x-direction), each layer starts to drag adjacent fluid layer but the effect of drag reduces as we go further away from the plate in y-direction. Finally, at some distance from the plate this drag effect disappears or becomes insignificant. This region where the velocity is changing or where the velocity gradients exists, is called the boundary layer region. The region beyond boundary layer where the velocity gradients are insignificant is called the potential flow region.



→ Boundary layer (keeps on growing with x)

Fig External flow over a flat plate

As depicted in Fig. 8.2, the boundary layer keeps growing along the x-direction, and may be referred to as the developing flow region. In internal flows (e.g. fluid flow through a pipe), the boundary layers finally merge after flow over a distance as shown in Fig. 8.3 below.



Fig Developing flow and fully developed flow region

The region after the point at which the layers merge is called the fully developed flow region and before this it is called the developing flow region. In fact, fully developed flow is another important assumption which is taken for finding solution for varity of fluid flow problem. In the fully developed flow region (as shown in Figure 8.3), the velocity vz is a function of r direction only. However, the developing flow region, velocity vz is also changing in the z direction.

Main axioms of transport phenomena

The basic equations of transport phenomena are derived based on following five axioms.

- Mass is conserved, which leads to the equation of continuity.
- Momentum is conserved, which leads to the equation of motion.
- Moment of momentum is conserved leads to an important result that the 2nd order stress tensor
 is symmetric.
- Energy is conserved, which leads to equation of thermal energy.
- Mass of component i in a multi-component system is conserved, which leads to the convective diffusion equation.

The solution of equations, resulting from axiom 2, 4 and 5 leads to the solution of velocity, temperature and concentration profiles. Ones these profiles are known, all other important information needed can be determined. We first take the axiom -1. Other axioms will be taken up one by one letter on.

There are three types of control volumes (CV) which may be chosen for deriving the equations based these axioms.

• Rectangular shaped control volume fixed in space

In this case, the control volume is rectangular volume element and is fixed in space. This method is the easiest to understand but requires more number of steps.

• Irregular shaped control volume element fixed in space

In this case, the control volume can be of any shape, but it is again fixed in space. This method is somewhat more difficult than the previous method as it requires little better understanding vector analysis and surface and volume integrals.

• Material volume approach

In this case, the control volume can be of any shape but moves with the velocity of the flowing fluid. This method is most difficult in terms of mathematics, but requires least number of steps for deriving the equations.

All three approaches when applied to above axiom, lead to the same equations. In this web course, we follow the first approach. Other approaches may be found elsewhere. Axioms-1

Mass is conserved

Consider a fluid of density ρ flowing with velocity \mathcal{X} as shown in Fig. 8.4. Here, ρ and \mathcal{X} are functions of space (x,y,z) and time (t). For conversion of mass, the rate of mass entering and leaving from the control volume (net rate of inflow) has to be evaluated and this should be equal to the rate of accumulation of mass in the control volume (CV). Thus, conservation of mass may be written in words as given below

 $\begin{pmatrix} \text{rate of accumulation of} \\ \text{mass in control volume} \end{pmatrix} = \begin{pmatrix} \text{rate of inflow of mass} \\ \text{into control volume} \end{pmatrix} - \begin{pmatrix} \text{rate of inflow of mass} \\ \text{out} \end{pmatrix}$



Fig 8.4 Fixed rectangular volume element through which fluid is flowing

The equation is then divided by the volume of the CV and converted into a partial differential equation by taking the limit as all dimensions go to zero. This limit effectively means that CV collapses to a point, thereby making the equation valid at every point in the system.

Let m and m+ Δ m be the mass of the control volume at time t and t+ Δ t respectively. Then, the rate of accumulation,

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

In order to evaluate the rate of inflow of mass into the control volume, we need to inspect how mass enters the control volume. Since the fluid velocity has three components vx, vy and vz, we need to identify the components which cause the inflow or the outflow at each of the six faces of the rectangular CV. For example, it is the component vx which forces the fluid to flow in the x direction, and thus it makes the fluid enter or exit through the faces having area $\Delta y \Delta z$ at x = x and $x = x + \Delta x$ respectively. The component vy forces the fluid in y direction, and thus it makes the fluid to flow in z direction, and thus it makes the fluid to flow in z direction, and thus it makes the fluid to flow in z direction, and thus it makes fluid enter or exit through the faces having area $\Delta x \Delta z$ at y = y and $y = y + \Delta y$ respectively. Similarly, the component vz forces the fluid to flow in z direction, and thus it makes fluid enter or exit through the faces having area $\Delta x \Delta y$ at z = z and $z = z + \Delta z$ respectively.

The rate mass entering in x direction through the surface $\Delta y \Delta z$ is $(\rho v x \Delta y \Delta z | x)$, the rate of mass entering in y direction through the surface $\Delta x \Delta z$ is $(\rho v y \Delta x \Delta z | y)$ and the rate of mass entering from z direction through the surface $\Delta x \Delta y$ is $(\rho v z \Delta x \Delta y | z)$. In a similar manner, expressions for the rate of mass leaving from the control volume may be written.

Thus, the conservation of mass leads to the following expressions

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

Dividing the Equation (8.1) by the volume $\Delta x \Delta y \Delta z$, we obtain

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

Note that each term in Equation (8.2) has the unit of mass per unit volume per unit time. Now, taking the limits $\Delta x \rightarrow 0$, $\Delta y \rightarrow 0$ and $\Delta z \rightarrow 0$, we get

$$\frac{\partial \rho}{\partial t} = \lim_{\Delta x \to 0} \left[\frac{(\rho v_x)|_x - (\rho v_x)|_{x + \Delta x}}{\Delta x} \right] + \lim_{\Delta y \to 0} \left[\frac{(\rho v_y)|_y - (\rho v_y)|_{y + \Delta y}}{\Delta y} \right] + \lim_{\Delta z \to 0} \left[\frac{(\rho v_y)|_y - (\rho v_y)|_{y + \Delta y}}{\Delta y} \right]$$

and using the definition of derivative, we finally obtain

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

Equation (8.4) is applicable to each point of the fluid. Rearranging the terms, we get the equation of continuity, may be written as given below.

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

We need not to derive the equation of continuity again and again in other coordinate system (that is, spherical or cylindrical). The idea is to rewrite Equation (8.5) in vector and tensor form. Once it is written in this form, the same equation may be applied to other coordinate system as well. Thus, the Equation (8.5) may be rewritten in vector and tensor form as shown below.

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

Vector and tensor analysis of cylindrical and spherical coordinate systems is not done here, and can be looked up elsewhere. Thus, the final expressions in cylindrical and spherical coordinates

are given as below.

cylindrical coordinates (r, θ , z)

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

Spherical coordinates (r, θ, ϕ)

$$\frac{\partial \rho}{\partial t} + \frac{1}{r^2} \frac{\partial}{\partial r} (\rho r v_r) + \frac{1}{r \sin \theta} \frac{\partial}{\partial \theta} (\rho v_\theta \sin \theta) + \frac{1}{r \sin \theta} \frac{\partial}{\partial \varphi} (\rho v_\varphi) = 0$$

Equation of continuity in terms of substantial derivative

The second term in Equation (8.6) may be broken into two parts as shown below. Partial derivative present in the Equation (8.6) can be converted into substantial derivative using vector and tensor identities.

$$\frac{\partial \rho}{\partial t} + \underline{y}.\nabla \rho + \rho \nabla \underline{y} = 0$$

In the above equation, the first two terms may be combined using the definition of substantial derivative to obtain the following equation.

$$\frac{D\rho}{Dt} + \rho \nabla \underline{v} = 0$$

In some cases, the fluid may be incompressible, i.e. density ρ is a constant with time as well as space coordinates. For example, water may be assumed as an incompressible fluid under isothermal conditions. In fact, all liquids may be assumed as incompressible fluids under isothermal conditions. For this special case, the equation of continuity may be further simplified as shown below

$$\nabla \underline{y} = 0$$
 (ρ is constant)

The above equation for an incompressible fluid does not mean that the system is under steady state conditions.



SCHOOL OF BIO & CHEMICAL ENGINEERING

DEPARTMENT OF CHEMICAL ENGINEERING

UNIT – III – Transport Phenomena for Bioprocesses – SCHA1511

1. Introduction to Heat Transfer

Practically all the operations that are carried out by the chemical engineers involve the production or absorption of energy in the form of heat. The study of temperature distribution and heat transfer is of great importance to engineers because of its almost universal occurrence in many branches of science and engineering. The first step in the optimal design of heat exchangers such as boilers, heaters, refrigerators and radiators is a detailed analysis of heat transfer. This is essential to determine the feasibility and cost of the undertaking, as well as the size of equipment required to transfer a specified amount of heat in a given time. Difference between thermodynamics and heat transfer Thermodynamic tells us (i) How much heat is transferred (ii) How much work is done (iii) Final state of the system.

Heat transfer tells us: (i) How much heat is transferred (with what modes) (ii) At what rate heat is transferred (iii) Temperature distribution inside the body.

The various modes of heat transfer are (i) conduction (ii) convection (iii) radiation. Conduction Heat transfer by the actual but invisible movement of molecules within the continuous substance due to temperature gradient is known as conduction. When a current or macroscopic particle of fluid crosses a specific surface, it carries with it a definite quantity of enthalpy. Such a flow of enthalpy is called convection. Convection is the mode of heat transfer in which the heat flow is associated with the movement of fluid. Transfer of energy through space by electromagnetic waves is known as radiation.

1.1 Applications of heat transfer

Energy production and conversion -steam power plant, solar energy conversion etc. Refrigeration and air-conditioning Domestic applications -ovens, stoves, toaster Cooling of electronic equipment Manufacturing / materials processing -welding, casting, soldering, laser machining Automobiles / aircraft design

1.1.1 Conduction: It is the transfer of internal energy by microscopic diffusion and collisions of particles or quasi-particles within a body due to a temperature gradient. The microscopically diffusing and colliding objects include molecules, electrons, atoms, and phonons. They transfer disorganized microscopic kinetic and potential energy, which are jointly known as internal energy. Conduction can only take place within an object or material, or between two objects that are in direct or indirect contact with each other. On a microscopic scale, heat conduction occurs as hot, rapidly moving or

vibrating atoms and molecules interact with neighboring atoms and molecules, transferring some of their energy (heat) to these neighboring particles. In other words, heat is transferred by conduction when adjacent atoms vibrate against one another, or as electrons move from one atom to another.

Fourier's law of heat Conduction

The rate of heat transfer due to conduction is governed by Fourier's Law, as shown

$$q = kA\left(\frac{\Delta T}{\Delta x}\right)$$

The terms in Eqn. 1 are:

q – rate of heat transfer (W)

k – thermal conductivity (W/m·K)

A – surface area across which heat is transferred (m^2)

 ΔT – difference in temperature over which heat is transferred (K)

 Δx – distance over which heat is transferred (m)

Thermal conductivity indicates the ease of heat transfer through a material and is a material dependent property. The ΔT term is the driving force for heat transfer.

1.1.2 Convection

The rate of heat transfer due to convection is described by

$$q = hA(\Delta T)$$

In Eqn. 2 the new term is:

h –heat transfer coefficient ($W/m^2 \cdot K$)

In Eqn. 2, the heat transfer coefficient replaces the $k/\Delta x$ term in Eqn. 1. The reason this happens is because convection has a mobile phase, and thickness is no longer an effective way of describing how the heat is transferred. The heat transfer coefficient can be thought of as the inverse of the resistance to heat transfer. Also, because temperature is a function of distance from a surface, the ΔT term is calculated between the surface and the bulk temperature of the mobile phase.

1.1.3 Radiation

The concept for radiation is that all materials are constantly emitting infrared radiation that is absorbed by other materials. For this module, we will assume that radiation is emitted directly outward from the surface of objects. While conduction and convection are driven by a temperature gradient, radiation is only based on the temperature of the object emitting radiation.

The rate of heat transfer due to radiation can be described by

Radiation Emitted:	$q_{out} = \varepsilon A \sigma(T_s^4)$
Radiation Absorbed:	$q_{in} = \alpha A \sigma (T_o^4)$

Heat transfer is the exchange of <u>thermal energy</u> between physical systems. The rate of <u>heat</u> transfer is dependent on the temperatures of the systems and the properties of the intervening medium through which the heat is transferred. The three fundamental modes of heat transfer are <u>conduction</u>, <u>convection</u> and <u>radiation</u>.

Heat transfer, the flow of energy in the form of heat, is a process by which a system changes its internal energy, hence is of vital use in applications of the First Law of Thermodynamics. Conduction is also known as diffusion, not to be confused with <u>diffusion</u> related to the mixing of constituents of a fluid. The direction of heat transfer is from a region of high temperature to another region of lower temperature, and is governed by the <u>Second Law of Thermodynamics</u>. Heat transfer changes the <u>internal energy</u> of the systems from which and to which the energy is transferred. Heat transfer will occur in a direction that increases the entropy of the collection of systems. <u>Thermal equilibrium</u> is reached when all involved bodies and the surroundings reach the same temperature. <u>Thermal expansion</u> is the tendency of matter to change in <u>volume</u> in response to a change in <u>temperature</u>.

Newton's law of cooling states that *the rate of heat loss of a body is proportional to the difference in temperatures between the body and its surroundings*. As such, it is equivalent to a statement that the <u>heat transfer coefficient</u>, which mediates between heat losses and temperature differences, is a constant. This condition is generally true in <u>thermal conduction</u> (where it is guaranteed by <u>Fourier's law</u>), but it is often only approximately true in conditions of <u>convective heat transfer</u>, where a number of physical processes make effective heat transfer coefficients somewhat dependent on temperature differences. Finally, in the case of heat transfer by <u>thermal radiation</u>, Newton's law of cooling is not true.

Thermal conductivity (often denoted k, λ , or κ) is the property of a material to <u>conduct heat</u>. It is evaluated primarily in terms of <u>Fourier's Law</u> for <u>heat conduction</u>. Heat transfer occurs at a lower rate across materials of low thermal conductivity than across materials of high thermal conductivity. Correspondingly, materials of high thermal conductivity are widely used in <u>heat sink</u> applications and materials of low thermal conductivity are used as <u>thermal insulation</u>. The thermal conductivity of a material may depend on temperature. The reciprocal of thermal conductivity is called thermal resistivity. Thermal conductivity is actually a <u>tensor</u>, which means it is possible to have different values in different directions.

Table 1: Thermal conductivity at room temperature for some metals and non-metals

	Metals		Ag	Cu	Al	Fe	Steel	
k [W/m-K]		420	390	200	70	50		
Non-m	etals	H20	Air	Engine oil	H2	Brick	Wood	Cork
k [W/n	n-K]	0.6	0.026	0.15	0.18	0.4 -0 .5	0.2	0.04

1.2 Effect of temperature on thermal conductivity

Thermal conductivity is the physical property of the substance. It depends upon temperature gradient. For pure metals, thermal conductivity decreases with an increase in temperature. For gases and insulators, thermal conductivity increases with an increase in temperature. For small ranges of temperature, k may be considered constant. For larger temperature ranges, thermal conductivity can be approximated by an equation of the form k = a + bT, where a and b are empirical constants.

Steady-State Conduction It is the form of conduction which happens when the temperature difference driving the conduction is constant so that after an equilibrium time, the spatial distribution of temperatures (temperature field) in the conducting object does not change any further. In steady state conduction, the amount of heat entering a section is equal to amount of heat coming out. Unsteady state conduction It is the form of conduction which happens when the temperature difference driving the conduction is not constant so that after an equilibrium time, the spatial distribution of temperatures (temperature field) in the conducting object changes as a function of time. Heat flux is denoted as q/A and it is defined as the rate of heat flow passing through a material per cross-sectional area and its unit is w/m².

Silver is the material which possess highest thermal conductivity and being a solid it is composed of

closed packing arrangement and due to this more molecular interactions within the molecules and hence the thermal conductivity is high.

Thermal conductivity is ability of a material to transport heat energy through it from high temperature region to low temperature region. The heat energy, Q, transported across a plane of area A in presence of a temperature gradient $\Delta T/\Delta I$ is given where k is the thermal conductivity of the material. It has units as W/m.K. It is a microstructure sensitive property. • Its value range o for metals 20-400 for ceramics 2-50 for polymers order of 0.3 Mechanisms - Thermal conductivity Heat is transported in two ways – electronic contribution, vibrational (phonon) contribution. In metals, electronic contribution is very high. Thus metals have higher thermal conductivities. It is same as electrical conduction. Both conductivities are related through Wiedemann-Franz law where L – Lorentz constant ($5.5x10^{-9}$ cal.ohm/sec.K²) • As different contributions to conduction vary with temperature, the above relation is valid to a limited extension for many metals. • With increase in temperature, both number of carrier electrons and contribution of lattice vibrations increase. Thus thermal conductivity of a metal is expected to increase. However, because of greater lattice vibrations, electron mobility decreases. The combined effect of these factors leads to very different behavior for different metals. Eg.: thermal conductivity of iron initially decreases then increases slightly; thermal conductivity decreases with increase in temperature for aluminium; while it increases for platinum.

1.3.1 HEAT TRANSFER THROUGH A PLANE WALL

Let us consider a plane wall of thickness L, thermal conductivity k, inside surface temperature Ti, outside surface temperature To. Let Q be the rate of heat transferred through the plane wall.

By Fourier's law of heat conduction

Q = -kA dT/dx



Fig. 1: Heat flow through a metal wall

$$Q \int_{0}^{L} dx = -k A \int_{T_{i}}^{T_{o}} dT$$

On integrating the above eqn, $Q = KA(T_i-T_o) / L$

 $Q = KA \Delta T / L$ i.e $Q = \Delta T / (KA/L)$ where $KA/L = R_{th}$ where R_{th-} thermal resistance measured in °C / Watts or K / Watts. Hence $Q = \Delta T / R_{th}$.

1.3.2 HEAT TRANSFER THROUGH A HOLLOW CYLINDER

Let us consider a hollow cylinder. The inside radius of the cylinder is r_1 , the outside radius is r_2 , and the length of the cylinder is L. The thermal conductivity of the material of which the cylinder is made is k. The temperature of the outside surface is T_2 , and that of the inside surface is T_1 .

By Fourier's law of heat conduction,



Fig. 2 Heat flow through a cylinder

Q = -kA dT/dr

$$Q \int_{r_1}^{r_2} \frac{dr}{r} = -k \ 2\pi L \int_{T_1}^{T_2} dT$$

integrating the above eqn,

$$Q = \frac{2\pi kL \left(T_1 - T_2\right)}{\ln\left(\frac{r_2}{r_1}\right)}$$

1.3.2.1 LOGARITHMIC MEAN RADIUS AND ARITHMETIC MEAN RADIUS

Logarithmic mean radius is the radius that when applied to the integrated equation for a flat wall, will give the correct rate of heat flow through a thick walled cylinder. It is given by the expression

$$\overline{r_{L}} = \frac{r_{o} - r_{i}}{\ln\left(\frac{r_{o}}{r_{i}}\right)}$$
where $\overline{r_{L}}$ is the logarithmic mean radius of the cylinder

 r_o is the outer radius of the pipe and

 r_i is the inner radius of the pipe.

Hence using the above expression $Q = 2\prod k L$ (Ti-To) * (ro-ri) / ln (ro/ri) *(ro-ri)

Using the Logarithmic mean radius expression in above, we get

 $Q=2\prod \; k \; L \; \; \Delta T \; {}^{*} \; r_{lm} \; / \; (\text{ro-ri}) \; \; \text{hence,} \; Q = \Delta T \; / \; (\text{ro-ri}) \; / \; A_{lm} \; {}^{*} \; k$

Where $A_{lm} = 2\prod L * r_{lm}$, A_{lm} is the logarithmic mean area which is used for thin cylinders.

1.3.3 COMPOUND RESISTANCES IN SERIES

(I) Heat Transfer Through A Composite Plane Wall

Let us consider a flat wall constructed of a series of 3 layers as shown. Let the thickness of the layers be L_1 , L_2 , L_3 and the average thermal conductivities of the materials of which the layers are made be k_1 , k_2 , k_3 respectively. Let us consider a hot fluid at a temperature T_a and heat transfer coefficient h_a inside the wall and cold fluid at a temperature T_b and heat transfer coefficient h_b outside the wall. Let T_1 , T_2 , T_3 and T_4 be the interface temperatures. It is desired to derive an equation for calculating the rate of heat flow through the series of resistances.





Rate of heat flow from the hot fluid to the inner surface of the wall

By Newton's law of cooling

 $\mathbf{Q} = \mathbf{h}_{a} \mathbf{A} \left(\mathbf{T}_{a} - \mathbf{T}_{b} \right)$

By rearranging the above eqn, we get

$$Q = \frac{(T_a - T_1)}{\frac{1}{h_a A}}$$

Rate of heat flow through the I layer, by Fourier's law of heat conduction,

 $Q = KA(T_1-T_2) / L$ On rearranging this,

$$Q = (T_1 - T_2) / (L_1 / K_1 . A)$$

Rate of heat flow through the II layer,

$$Q = (T_2 - T_3) / (L_2 / K_2 . A)$$

Rate of heat flow through the III layer,

$$Q = (T_3 - T_4) / (L_3 / K_3 . A)$$

Rate of heat flow from outer surface of the wall to the cold fluid By Newton's law of cooling $Q=h_b\;A\;(T_4-T_b)$ and $Q=(T_4-T_b)\;/\;1/\;h_b\;A$

Overall rate of heat flow =overall thermal resistance / overall temperature drop

Overall rate of heat flow

$$Q = \frac{(T_a - T_b)}{\frac{1}{h_a A} + \frac{L_1}{k_1 A} + \frac{L_2}{k_2 A} + \frac{L_3}{k_3 A} + \frac{1}{h_b A}}$$

In steady state heat conduction through a composite wall, this can be written as

 $Q = (T_1 - T_4) / (L_1/K_1.A + L_2/K_2.A + L_3/K_3.A)$

i.e Q = $\Delta T / R_{th1} + R_{th2} + R_{th3}$

Hence, $Q = \Delta T / \sum R_{th}$



Table 2 Various flows and their driving forces

Flow	Driving force
Electricity flow	Electric potential gradient
Fluid flow	Pressure gradient
Heat flow	Temperature gradient

It was observed in the previous discussion that for the given plane wall the area for heat transfer was constant along the heat flow direction. The plane solid wall was one of the geometries but if we take some other geometry (tapered plane, cylindrical body, spherical body etc.) in which the area changes in the direction of heat flow. Now we will consider geometrical configuration which will be mathematically simple and also of great engineering importance like hollow cylinder and hollow sphere. In these cases the heat transfer area varies in the radial direction of heat conduction. We will take up both the cases one by one in the following sections.

1.4) Heat transfer through co-axial cylinder Provided with one layer of insulation



Fig. 4 Heat flow through a composite cylinder

Let us consider coaxial cylinders constructed of a series of 3 layers as shown in fig. Let $R_0 R_1$ and R_2 be the radii of the cylinders and the average thermal conductivities of the materials of which the layers are made be k_1 and k_2 respectively. Let us consider a hot fluid at a temperature T_b and heat transfer coefficient h_b inside the cylinder and cold fluid at a temperature T_a and heat transfer coefficient h_a outside the cylinder. Let T_o , T_1 and T_2 be the interface temperatures. It is desired to derive an equation for calculating the rate of heat flow through the composite cylinder provided with series of resistances.

Consider a very thin hollow cylinder of thickness d_r in the main geometry (fig.2.9a) at a radial distance r. If d_r is small enough with respect to r, then the area of the inner and outer surface of the thin cylinder may be considered to be of same area. In other words, for very small d_r with respect to r, the lines of heat flow may be considered parallel through the differential element in radial outward direction.

We may ignore the heat flow through the ends if the cylinder is sufficiently large. We may thus eliminate any dependence of the temperature on the axial coordinate and for one dimensional steady state heat conduction, the rate of heat transfer for the thin cylinder,

$$\dot{q} = -k \frac{dT}{dr} \ 2\pi r L$$

Where dT is the temperature difference between the inner and outer surface of the thin cylinder considered above and k is the thermal conductivity of the cylinder. On rearranging,

$$\frac{dr}{r} = -\frac{2\pi Lk}{\dot{q}} dT$$

To get the heat flow through the thick wall cylinder, the above equation can be integrated between the limits,

$$\int_{r_i}^{r_o} \frac{dr}{r} = -\frac{2\pi Lk}{\dot{q}} \int_{T_i}^{T_o} dT$$

On solving,

$$\dot{q} = k(2\pi L) \frac{(T_i - T_o)}{\ln(r_o/r_i)}$$
$$\dot{q} = kA_{LM} \frac{(T_i - T_o)}{r_o - r_i}$$

Rate of heat flow from the hot fluid to the inner surface of the wall

By Newton's law of cooling,

$$\mathbf{Q} = \mathbf{h}\mathbf{b} \mathbf{A} \left(\mathbf{T}_{\mathbf{b}} - \mathbf{T}_{\mathbf{0}}\right)$$

 $Q = hb \ 2 \prod RL \ (T_b - T_o)$

By rearranging the above,

$$Q = (Tb - To) / 1 / 2\pi R_o L$$

Rate of the heat flow through the cylinder By Fourier's law of heat conduction

$$Q = \frac{2\pi kL \left(T_1 - T_2\right)}{\ln\left(\frac{r_2}{r_1}\right)}$$

using the above conditions from the fig,

$$Q = 2\prod k_1 L (T_0 - T_1) / \ln (R_1/R_0)$$

By rearranging the above,

 $Q = (T_o - T_1) / ln (R_1/R_o) / 2 \prod k_1 L$

Rate of the heat flow through the II layer By Fourier's law of heat conduction

$$Q = (T_1 - T_2) / \ln (R_2/R_1) / 2 \prod k_2 L$$

Rate of heat flow from the outer surface of the wall to the cold fluid

By Newton's law of cooling

$$\mathbf{Q} = \mathbf{ha} \mathbf{A} \left(\mathbf{T2} - \mathbf{Ta} \right)$$

Q = ha $2\pi R_2 L~(T2-Ta)$ on rearranging, Q = (T2-Ta) / 1 / ha $2\prod R_2 L$

Overall rate of heat flow = overall thermal resistance / overall temperature drop

Hence overall rate of heat flow is given by

$$Q = (T_b - T_a) / (1/hb \ 2 \Box \ R_o) + (\ln (R_1/R_o) / 2 \prod k_1 L) + (\ln (R_2/R_1) / 2 \prod k_2 L) + (1/ha \ 2 \prod R_2 L)$$

For steady state conduction, heat transfer coefficients can be neglected and the heat flow is given by

$$Q = (T_b - T_a) / (\ln (R_1/R_o) / 2 \prod k_1 L) + (\ln (R_2/R_1) / 2 \prod k_2 L)$$

Hence $Q = \Delta T / R_{th1} + R_{th2}$

Where $R_{th1} = (\ln (R_1/R_0) / 2 \prod k_1 L)$ and $R_{th2} = (\ln (R_2/R_1) / 2 \prod k_2 L)$

$$Q = \Delta T / \sum R_{th}$$

1.5 Insulation

The addition of insulation material on a surface reduces the amount of heat flow to the ambient. There are certain instances in which the addition of insulation to the outside surface of cylindrical of spherical walls does not reduce the heat loss. Under certain circumstances it actually increases the heat loss up to a certain thickness of insulation. It is well known fact that the rate of heat transfer will approach zero if an infinite amount of insulation are added. This means that there must be a value of radius for which rate of heat transfer is maximum. This value is known as the critical radius of insulation, rc.

Variation of thermal conductivity with respect to solids, liquids and gases

In solids, solids, heat conduction conduction is due to two effects effects: the lattice lattice vibrational vibrational waves induced by the vibrational motions of the molecules positioned at relatively fixed positions in a periodic manner called a lattice, and the energy transported via the free flow of electrons in the solid. • The thermal conductivity of a solid is obtained by adding the lattice and electronic components. The relatively high thermal conductivities of pure metals are primarily due to the electronic component. The lattice component of th l erma cond ii uct v ty strongly d d epen s on the way the molecules are arranged. For example, diamond, which is a highly ordered crystalline solid has the highest known thermal conductivity at room. Conduction crystalline solid, has the highest known thermal conductivity at room temperature.

The thermal thermal conductivities conductivities of materials materials vary with temperature temperature. The variation of thermal conductivity over certain temperature ranges is negligible for some materials, but significant for others. The thermal conductivities of certain solids exhibit dramatic increases at temperatures near absolute zero, when these solids become superconductors.

5.1 CRITICAL RADIUS OF INSULATION IN PIPES

Let us consider an insulating layer in the form of a hollow cylinder of length L. Let ri and ro be the inner and outer radii of insulation. The thermal conductivity of the material of which the layer is made be k. Let the inside surface of insulation be at a temperature Ti, and the outside surface at a temperature To be dissipating heat by convection to the surroundings at a temperature Tb with a heat transfer coefficient h. Then the rate of heat transfer Q through this insulation layer is



Fig. 5 Heat flow through a cylindrical pipe for critical radius

$$Q = \frac{2\pi L \left(T_i - T_b\right)}{\frac{\ln\left(\frac{r_o}{r_i}\right)}{k} + \frac{1}{hr_o}}$$
(1)

The value of critical radius r_c , that is r_o for which Q is a maximum may be obtained by equating dQ/dr_o to zero.

$$\frac{dQ}{dr_o} = \frac{0 - (T_i - T_b) \left[\frac{1}{2\pi k L r_o} - \frac{1}{2\pi h L r_o^2} \right]}{\left[\frac{\ln\left(\frac{r_o}{r_i}\right)}{2\pi k L} + \frac{1}{2\pi h L r_o} \right]^2}$$
(2)

 $(T_i - T_b) \neq 0$ (Since it is the driving force)

$$\therefore \quad \frac{1}{2\pi k L r_o} - \frac{1}{2\pi h L r_o^2} = 0 \tag{3}$$

$$r_0 = \frac{k}{h} = r_c$$

The radius at which the rate of heat transfer is maximum is known as the critical radius of insulation.

1.6 VARIABLE THERMAL CONDUCTIVITY

Let us a hollow cylinder. The inside radius of the cylinder is ri, the outside radius is ro, and the length of the cylinder is L. The thermal conductivity of the material of which the cylinder is varies with temperature as $k = ko(1 + \alpha T)$. The temperature of the outside surface is To and that of the inside surface is Ti. This can be used with many equations such as

$$k = ko (\alpha + \beta T)$$

$$k = ko (\alpha + \beta T + \gamma T^{2})$$

$$k = ko (a + bT)$$

$$k = ko (a + bT + cT^{2})$$

By Fourier's law of heat conduction

$$Q = -kA \frac{dT}{dr}$$
(1)

$$Q = -k_{o} (1 + \beta T) A \frac{dT}{dr}$$

$$Q \int_{r}^{r_{o}} \frac{dr}{r} = -k_{o} 2\pi L \int_{T}^{T_{o}} (1 + \beta T) dT$$
(2)

$$\mathsf{Q} \ln \frac{r_o}{r_i} = k_0 2\pi L \left(1 + \beta \frac{\left[T_i + T_o\right]}{2} \right) \left(T_i - T_o\right)$$

$$Q = \frac{k_0 2\pi L \left(1 + \beta \frac{\left[T_i + T_o\right]}{2}\right) (T_i - T_o)}{\ln \frac{r_o}{2}}$$
(3)

1.7 Introduction to Unsteady state heat transfer

A solid body is said to be in a steady state if its temperature does not vary with time. If however there is an abrupt change in its surface temperature or environment it takes some time before the body to attain an equilibrium temperature or steady state. During this interim period the temperature varies with time and the body is said to be in an unsteady or transient state. The analysis of unsteady state heat transfer is of great interest to engineers because of its widespread occurrence such as in boiler tubes, rocket nozzles, automobile engines, cooling of IC engines, cooling and freezing of food, heat treatment of metals by quenching, etc. For practical purposes it is necessary to know the time taken to attain a certain temperature when the environment suddenly changes. The solution of an unsteady sate problem will be more complex than that of steady state one because of the presence of another variable time, t. Transient heat conduction problems can be divided into periodic heat flow and non periodic heat flow problems. Periodic heat flow problems are those in which the temperature varies on a regular basis, eg., the variation of temperature of the surface of the earth during a twenty four hour period.. In the non periodic type, the temperature at any point within the system varies non linearly with time.

Introduction to this point, we have considered conductive heat transfer problems in which the temperatures are independent of time. In many applications, however, the temperatures are varying with time, and we require the understanding of the complete time history of the temperature variation. For example, in metallurgy, the heat treating process can be controlled to directly affect the characteristics of the processed materials. Annealing (slow cool) can soften metals and improve ductility. On the other hand, quenching (rapid cool) can harden the strain boundary and increase strength. In order to characterize this transient behavior, the full unsteady equation is needed.

$$\frac{1}{a} \cdot \frac{\partial T}{\partial \tau} = \frac{\partial^2 T}{\partial x^2} + \frac{\partial^2 T}{\partial y^2} + \frac{\partial^2 T}{\partial z^2} + \frac{q}{k}$$

Where $\alpha = \frac{k}{\rho c}$ is the thermal diffusivity. Without any heat generation and considering spatial variation of temperature only in x-direction, the above equation reduces to:

1.8 Systems with negligible internal resistance – Lumped Heat Analysis

Heat transfer in heating and cooling of a body is dependent upon both the internal and surface resistances. The simplest unsteady state problem is one in which the internal resistance is negligible, that is, the convective resistance at the surface boundary is very large when compared to the internal resistance due to conduction. In other words, the solid has an infinite thermal conductivity so that there is no variation of temperature inside the solid and temperature is a function of time only. This situation cannot exist in reality because all the solids have a finite thermal conductivity and there will always be a temperature gradient inside whenever heat is added or removed. Problems such as heat treatment of metals by

quenching, time response of thermocouples and thermometers, etc can be analyzed by this idealization of negligible internal resistance. The process in which the internal resistance is ignored being negligible in comparison with its surface resistance is called the Newtonian heating and cooling process. In Newtonian heating and cooling process the temperature throughout the solid is considered to be uniform at a given time. Such an analysis is called the lumped heat capacity analysis.

1.9 Systems with negligible surface resistance

Another class of transient problems met with in practice is one in which the surface resistance is negligible compared to the overall resistance. This amounts to saying that the convective heat transfer coefficient at the surface is infinity. For such a process the surface temperature remains constant for all the time and its value is equal to that of ambient temperature.

Dimensionless parameters:

$$\frac{T_i - T_s}{T_s - T_{\infty}} = \frac{\overline{hL}}{k} = \text{Biot number}$$

$Bi = \frac{resistance \text{ to internal heat flow}}{resistance \text{ to external heat flow}}$

The Biot number is dimensionless, and it can be thought of as the ratio to the internal and external heat flows. Whenever the Biot number is small, the internal temperature gradients are also small and a transient problem can be treated by the "lumped thermal capacity" approach. The lumped capacity assumption implies that the object for analysis is considered to have a single mass-averaged temperature.

In general, a characteristic length scale may be obtained by dividing the volume of the solid by its surface area: $L = V/A_s$

Using this method to determine the characteristic length scale, the corresponding Biot number may be evaluated for objects of any shape, for example a plate, a cylinder, or a sphere. As a thumb rule, if the Biot number turns out to be less than 0.1, lumped capacity assumption is applied. In this context, *a dimensionless time*, known as the Fourier number, can be obtained by multiplying the dimensional time by the thermal diffusivity and dividing by the square of the characteristic length:

dimensionless time = $\frac{\alpha t}{L^2} = Fo$

Lumped heat capacity

analysis: temperature distribution inside or outside the solid is neglected.

The cases considered so far have been those in which the heat conducting solid is free of internal heat generation. However, the situations where the internal heat is generated are very common cases in chemical industries for example, the exothermic reaction in the solid pallet of a catalyst.

We have learnt that how the Fourier equation is used for the steady-state heat conduction through the composites of three different geometries that were not having any heat source in it. However, the heat generation term would come into the picture for these geometries. It would not be always easier to remember and develop heat conduction relations for different standard and non-standard geometries. Therefore, at this point we should learn how to develop a general relation for the heat conduction that should be applicable to the entire situation such as steady-state, unsteady state, heat source, different geometry, heat conduction in different direction, etc. Again here we will consider that the solid is isotropic in nature, which means the thermal conductivity of the material is same in all the direction of heat flow.

To get such a general equation the differential form of the heat conduction equation is most important. For simplicity, we would consider an infinitesimal volume element in a Cartesian coordinate system. The dimensions of the infinitesimal volume element are d_x , d_y , and d_z in the respective direction as shown in the fig
The simplest situation in an unsteady heat transfer process is to use the lump assumption, wherein we neglect the temperature distribution inside the solid an with the heat transfer between the solid and the ambient fluids. In other wc assuming that the temperature inside the solid is constant and is equal to temperature.



Fig. 6

The solid object shown in figure 5.2 is a metal piece which is being cooled in forming. Thermal energy is leaving the object from all elements of the surface shown for simplicity by a single arrow. The first law of thermodynamics approblem is

 $\begin{pmatrix} \text{heat out of object} \\ \text{during time } dt \end{pmatrix} = \begin{pmatrix} \text{decrease of internal thermal} \\ \text{energy of object during time } dt \end{pmatrix}$

Now, if Biot number is small and temperature of the object can be considered to this equation can be written as

$$\overline{h}A_{s}[T(t) - T_{\infty}]dt = -\rho c V dT$$

or,

$$\frac{dT}{(T-T_{\infty})} = -\frac{\overline{h}A_s}{\rho cV}dt$$

Integrating and applying the initial condition $T(0) = T_i$,

$$\ln \frac{T(t) - T_{\infty}}{T_t - T_{\infty}} = -\frac{\overline{h}A_s}{\rho c V}t$$

Taking the exponents of both sides and rearranging,

$$\frac{T(t) - T_{\infty}}{T_t - T_{\infty}} = e^{-bt}$$

where

$$b = \frac{\overline{h}A_s}{\rho cV} \qquad (1/s)$$

b is a positive quantity having dimension (time)-1. The reciprocal of *b* is usually called *time constant*, which has the dimension of time.

1.10 Heat conduction through spherical surface 6

Heat Conduction in a Spherical Shell



Fig. 7 Heat flow through a spherical surface

Consider a spherical shell with inside radius r_1 and outside radius r_2 . Let T_1 be the inside temperature and T_2 be the outside temperature. K be the thermal conductivity of the material. Q be the heat flow through the spherical shell with a cross sectional area to be A. based on Fourier's law of heat conduction and following the assumptions,

- (i) Heat flow is uniform
- (ii) Heat flow is normal to the surface
- (iii) The material is uniform and possess constant thermal conductivity
- (iv) Heat flow is uni-directional

Let us consider a differential element of thickness dr which is lying between inside and outside radius. For such an element the heat flow is given by

Q = -kA dT/dr where area of the sphere is $A = 4\pi r^2$

Substituting the area of a sphere

Integrating, between $r = r_1$ and r_2 , and T_1 and T_2 ,

$$\frac{q_r}{4\pi} \left| -\frac{1}{r} \right|_{r_1}^{r_2} = -k \left| T \right|_{T_1}^{T_2}$$

$$\frac{q_r(r_2 - r_1)}{4\pi r_1 r_2} = -k(T_2 - T_1)$$

$$q_r = \frac{4\pi k r_1 r_2 (T_1 - T_2)}{(r_2 - r_1)}$$

The thermal resistance is expressed as

 $Q = \Delta T / (r_2 - r_1) / 4\pi k r_1 r_2$ where the resistance is given by $(r_2 - r_1) / 4\pi k r_1 r_2$ Geometric mean radius is given by $r_m^2 = r_1 r_2$ and hence $R_{th} = (r_2 - r_1) / A_m$. k where $A_m = 4\pi r_m^2$ and A_m is the geometric mean area.

Similarly, rate of heat flow for a composite spherical shell with one layer of insulation is given by

$$Q = \Delta T / [(r_2 - r_1) / 4\pi k_1 r_1 r_2 + (r_3 - r_2) / 4\pi k_2 r_2 r_3]$$

In a plane wall the area perpendicular to the direction of heat flow adding more insulation to a wall always decreases heat transfer. If thicker is insulation, the lower is the heat transfer rate. This is due to the fact the outer surface have always the same area. But in cylindrical and spherical coordinates, the addition of insulation also increases the outer surface, which decreases the convection resistance at the outer surface. Moreover, in some cases, a decrease in the convection resistance due to the increase in surface area can be more important than an increase in conduction resistance due to thicker insulation. As a result the total resistance may actually decrease resulting in increased heat flow. The thickness upto which heat flow increases and after which heat flow decreases is termed as critical thickness. In the case of cylinders and spheres it is called critical radius. It can be derived the critical radius of insulation depends on the thermal conductivity of the insulation k and the external convection heat transfer coefficient h.

Optimum thickness of insulation

The radius of insulation at which the total annual cost is minimum corresponds to optimum thickness of insulation.

P.No. 1. A furnace wall consists of two layers, 22.5cm of fire brick(k=1.2kcal/hr m $^{\circ}$ C) and 12.5cm of insulating brick (k=0.15kcal/hr m $^{\circ}$ C). The temperature inside the furnace is 1650 $^{\circ}$ C and the inside heat transfer coefficient is 60kcal/hr m $^{\circ}$ C. The temperature of the surrounding atmosphere is 27 $^{\circ}$ C and the outside heat transfer coefficient is 10kcal/hr m 2 $^{\circ}$ C. Determine the rate of heat of loss per square meter of the wall.

Solution:

L₁ - 22.5 x 10⁻² m L₂ - 12.5 x 10⁻² m k₁ - 1.2 kcal/hr m °C k₂ - 0.15 kcal/hr m °C h_a - 60 kcal/hr m² °C h_b - 10kcal/hr m² °C T_a - 1650 °C T_b - 27 °C Q = $\frac{(T_a - T_b)}{\frac{1}{h_a A} + \frac{L_1}{k_1 A} + \frac{L_2}{k_2 A} + \frac{1}{h_b A}}$

$$Q / A = 1426.8 W / m^2$$

P.No.2. A pipe carrying steam at 220 °C has an I.D. of 15cm. The convection coefficient on the inside wall is $60W/m^2K$. The pipe wall thickness is 15mm and the thermal conductivity is 35W/mK. The outside is exposed to a chemical at 130°C with a convection coefficient of $15W/m^2K$. If the pipe wall is covered with two insulation layers, the first 3cm thickness with k=0.12W/mK and the second 4cm thickness with k= 0.35W/m K. Determine the rate of heat transfer.

Solution :

- r₁ 75 x 10⁻³ m
- r₂ 90 x 10⁻³ m
- r₃ 120 x 10⁻³ m
- r₄ 160 x 10⁻³ m
- k1 35 W / m K



1.11 Analogy between heat flow and electricity:

Heat flow is represented by Fourier's law of heat conduction whereas electrical flow is represented by ohm's law.

Heat flow = Temperature gradient / thermal resistance

Ohm's law is given by

Electrical flow = voltage drop / electrical resistance

The various parameters analogous to each other in both the laws are heat flow and electrical flow, voltage drop with temperature gradient, thermal and electrical resistance.



SCHOOL OF BIO & CHEMICAL ENGINEERING

DEPARTMENT OF CHEMICAL ENGINEERING

UNIT – IV – Transport Phenomena for Bioprocesses – SCHA1511

3.1 Introduction of Mass Transfer

When a system contains two or more components whose concentrations vary from point to point, there is a natural tendency for mass to be transferred, minimizing the concentration differences within a system. The transport of one constituent from a region of higher concentration to that of a lower concentration is called mass transfer.

The transfer of mass within a fluid mixture or across a phase boundary is a process that plays a major role in many industrial processes. Examples of such processes are:

- (i) Dispersion of gases from stacks
- (ii) Removal of pollutants from plant discharge streams by absorption
- (iii) Stripping of gases from waste water
- (iv) Neutron diffusion within nuclear reactors

(v) Air conditioning

Many of air day-by-day experiences also involve mass transfer, for example:

- A lump of sugar added to a cup of coffee eventually dissolves and then eventually diffuses to make the concentration uniform.
- (ii) Water evaporates from ponds to increase the humidity of passing-air-stream
- (iii) Perfumes present a pleasant fragrance which is imparted throughout the surrounding atmosphere.

The mechanism of mass transfer involves both molecular diffusion and convection.

3.2 Properties of Mixtures

Mass transfer always involves mixtures. Consequently, we must account for the variation of physical properties which normally exist in a given system. When a system contains three or more components, as many industrial fluid streams do, the problem becomes unwidely very quickly. The conventional engineering approach to problems of multicomponent system is to attempt to reduce them to representative binary (i.e., two component) systems.

In order to understand the future discussions, let us first consider definitions and relations which are often used to explain the role of components within a mixture.

3.2.1 Concentration of Species:

Concentration of species in multicomponent mixture can be expressed in many ways. For species A, mass concentration denoted by ρ_A is defined as the mass of A,m_A per unit volume of the mixture.

$$\rho_A = \frac{m_A}{V} \qquad \dots \qquad (1)$$

The total mass concentration density ρ is the sum of the total mass of the mixture in unit volume:

$$\rho = \sum_{i} \rho_{i}$$

where ρ_i is the concentration of species i in the mixture.

Molar concentration of, A, C_A is defined as the number of moles of A present per unit volume of the mixture.

By definition,

Numberof moles =
$$\frac{massof A}{molecularweightof A}$$

$$n_A = \frac{m_A}{M_A} \qquad \dots \qquad (2)$$

Therefore from (1) & (2)

$$C_A = \frac{n_A}{V} = \frac{\rho_A}{M_A}$$

For ideal gas mixtures,

$$n_A = \frac{p_A V}{R T}$$
 [from Ideal gas law PV = nRT]

$$C_A = \frac{n_A}{V} = \frac{p_A}{RT}$$

where p_A is the partial pressure of species A in the mixture. V is the volume of gas, T is the absolute temperature, and R is the universal gas constant.

The total molar concentration or molar density of the mixture is given by

$$C = \sum_{i} C_{i}$$

3.2.2 Velocities

In a multi-component system the various species will normally move at different velocities; and evaluation of velocity of mixture require the averaging of the velocities of each species present.

If v_{I} is the velocity of species i with respect to stationary fixed coordinates, then massaverage velocity for a multicomponent mixture defined in terms of mass concentration is,

$$v = \frac{\sum_{i} \rho_{i} v_{i}}{\sum_{i} \rho_{i}} = \frac{\sum_{i} \rho_{i} v_{i}}{\rho}$$

By similar way, molar-average velocity of the mixture v * is

$$v^* = \frac{\sum_{i} C_i V_i}{C}$$

For most engineering problems, there will be title difference in v * and v and so the mass average velocity, v, will be used in all further discussions.

The velocity of a particular species relative to the mass-average or molar average velocity is termed as diffusion velocity

(i.e) Diffusion velocity = $v_i - v_j$

The mole fraction for liquid and solid mixture, x_A , and for gaseous mixtures, y_A , are the molar concentration of species A divided by the molar density of the mixtures.

$$X_A = \frac{C_A}{C}$$
 (liquids and solids)

$$y_A = \frac{C_A}{C}$$
 (gases).

The sum of the mole fractions, by definition must equal 1;

(i.e.)
$$\sum_{i} x_{i} = 1$$
$$\sum_{i} y_{i} = 1$$

by similar way, mass fraction of A in mixture is;

$$W_A = \frac{\rho_A}{\rho}$$

10. The molar composition of a gas mixture at 273 K and 1.5 * 10 5 Pa is:

- O₂ 7%
- CO 10%
- CO₂ 15%
- N₂ 68%

Determine

- a) the composition in weight percent
- b) average molecular weight of the gas mixture
- c) density of gas mixture
- d) partial pressure of O₂.

Calculations:

Let the gas mixture constitutes 1 mole. Then

- O₂ = 0.07 mol
- CO = 0.10 mol
- CO₂ = 0.15 mol
- N₂ = 0.68 mol

Molecular weight of the constituents are:

O₂ = 2 * 16 = 32 g/mol CO = 12 + 16 = 28 g/mol CO₂ = 12 + 2 * 16 = 44 g/mol N₂ = 2 * 14 = 28 g/mol

Weight of the constituents are: (1 mol of gas mixture)

- O₂ = 0.07 * 32 = 2.24 g
- CO = 0.10 * 28 = 2.80 g
- CO₂ = 0.15 * 44 = 6.60 g
- N₂ = 0.68 * 28 = 19.04 g

Total weight of gas mixture = 2.24 + 2.80 + 6.60 + 19.04

= 30.68 g

Composition in weight percent:

$$O_2 = \frac{2.24}{30.68} * 100 = 7.30\%$$
$$CO = \frac{2.80}{30.68} * 100 = 9.13\%$$
$$CO_2 = \frac{6.60}{30.68} * 100 = 21.51\%$$

$$N_2 = \frac{19.04}{30.68} * 100 = 62.06\%$$

Average molecular weight of the gas mixture $M = \frac{\text{Weight of gas mixture}}{\text{Number of moles}}$

$$M = \frac{30.68}{1} = 30.68 \ g/mol$$

Assuming that the gas obeys ideal gas law,

$$\frac{n}{V} = \frac{P}{RT}$$

$$\frac{n}{V}$$
 = molar density = ρ_m

Therefore, density (or mass density) = $\rho_m M$

Where M is the molecular weight of the gas.

Density =
$$\rho_m M = \frac{PM}{RT} = \frac{1.5 * 10^5 * 30.68}{8314 * 273} kg/m^3$$

= 2.03 kg/m³

Partial pressure of O_2 = [mole fraction of O_2] * total pressure

$$= \frac{7}{100} * (1.5 * 10^{5})$$
$$= 0.07 * 1.5 * 10^{5}$$
$$= 0.105 * 10^{5} Pa$$

3.3 Diffusion flux

Just as momentum and energy (heat) transfer have two mechanisms for transport-molecular and convective, so does mass transfer. However, there are convective fluxes in mass transfer, even on a molecular level. The reason for this is that in mass transfer, whenever there is a driving force, there is always a net movement of the mass of a particular species which results in a bulk motion of molecules. Of course, there can also be convective mass transport due to macroscopic fluid motion. In this chapter the focus is on molecular mass transfer.

The mass (or molar) flux of a given species is a vector quantity denoting the amount of the particular species, in either mass or molar units, that passes per given increment of time through a unit area normal to the vector. The flux of species defined with reference to fixed spatial coordinates, N_A is

$$N_A = C_A \nu_A$$
(1)

This could be written interms of diffusion velocity of A, (i.e., $v_A - v$) and average velocity of mixture, v, as

$$N_{A} = C_{A} (v_{A} - v) + C_{A} v$$
 ------(2)

By definition

$$v = v^* = \frac{\sum_{i} C_{i} v_{i}}{C}$$

Therefore, equation (2) becomes

$$N_A = C_A (v_A - v) + \frac{C_A}{C} \sum_i C_i v_i$$

$$= C_A (v_A - v) + y_A \sum_i C_i v_i$$

For systems containing two components A and B,

The first term on the right hand side of this equation is diffusional molar flux of A, and the second term is flux due to bulk motion.

3.3.1 Fick's law:

An empirical relation for the diffusional molar flux, first postulated by Fick and, accordingly, often referred to as Fick's first law, defines the diffusion of component A in an isothermal, isobaric system. For diffusion in only the Z direction, the Fick's rate equation is

$$J_A = -D_{AB} \frac{dC_A}{dZ}$$

where D $_{AB}$ is diffusivity or diffusion coefficient for component A diffusing through component B, and dC_A / dZ is the concentration gradient in the Z-direction.

A more general flux relation which is not restricted to isothermal, isobasic system could be written as

$$J_A = -C D_{AB} \frac{d y_A}{dZ} \qquad -----(4)$$

using this expression, Equation (3) could be written as

$$N_{A} = -C D_{AB} \frac{d y_{A}}{d Z} + y_{A} N$$
 ------(5)

3.3.2 Relation among molar fluxes:

For a binary system containing A and B, from Equation (5),

$$N_{A} = J_{A} + y_{A}N$$

or
$$J_{A} = N_{A} + y_{A}N \qquad (6)$$

Similarly,

$$J_B = N_B + y_B N \quad \dots \quad \dots \quad (7)$$

Addition of Equation (6) & (7) gives,

$$J_{A} + J_{B} = N_{A} + N_{B} - (y_{A} + y_{B})N$$
(8)

By definition $N = N_A + N_B$ and $y_A + y_B = 1$.

Therefore equation (8) becomes,

$$\mathbf{J}_{\mathbf{A}} + \mathbf{J}_{\mathbf{B}} = \mathbf{0}$$
$$\mathbf{J}_{\mathbf{A}} = -\mathbf{J}_{\mathbf{B}}$$

From y_A + y_B = 1 dy_A = - dy_B

Therefore Equation (9) becomes,

This leads to the conclusion that diffusivity of A in B is equal to diffusivity of B in A.

3.4 Diffusivity

Fick's law proportionality, D _{AB}, is known as mass diffusivity (simply as diffusivity) or as the diffusion coefficient. D _{AB} has the dimension of L ² / t, identical to the fundamental dimensions of the other transport properties: Kinematic viscosity, $v\eta = (\mu / \rho)$ in momentum transfer, and thermal diffusivity, $\alpha (= k / \rho C_{\rho})$ in heat transfer.

Diffusivity is normally reported in cm² / sec; the SI unit being m² / sec.

Diffusivity depends on pressure, temperature, and composition of the system.

In table, some values of D_{AB} are given for a few gas, liquid, and solid systems.

Diffusivities of gases at low density are almost composition independent, incease with the temperature and vary inversely with pressure. Liquid and solid diffusivities are strongly concentration dependent and increase with temperature.

General range of values of diffusivity:

Gases :	5 X 10 ⁻⁶	 1 X 10 ⁻⁵	m² / sec.
Liquids :	10 -6	 10 ⁻⁹	m² / sec.
Solids :	5 X 10 ⁻¹⁴	 1 X 10 ⁻¹⁰	m ² / sec.

In the absence of experimental data, semitheoretical expressions have been developed which give approximation, sometimes as valid as experimental values, due to the difficulties encountered in experimental measurements.

3.4.1 Diffusivity in Gases:

Pressure dependence of diffusivity is given by

$$D_{AB} \propto \frac{1}{p}$$
 (for moderate ranges of pressures, upto 25 atm).

And temperature dependency is according to

$$D_{AB} \propto T^{\frac{3}{2}}$$

Diffusivity of a component in a mixture of components can be calculated using the diffusivities for the various binary pairs involved in the mixture. The relation given by Wilke is

$$D_{1-mixture} = \frac{1}{\frac{y'_2}{D_{1-2}} + \frac{y'_3}{D_{1-3}} + \dots + \frac{y'_n}{D_{1-n}}}$$

Where D _{1-mixture} is the diffusivity for component 1 in the gas mixture; D _{1-n} is the diffusivity for the binary pair, component 1 diffusing through component n; and y'_n is the mole fraction of component n in the gas mixture evaluated on a component -1 – free basis, that is

$$y'_2 = \frac{y_2}{y_2 + y_3 + \dots + y_n}$$

$$D_2m = \frac{1.847}{1.2 \times 10^5} = 1.539 \times 10^{-5} m^2/\text{sec}$$

By Similar calculations Diffusivity of N $_2$ in the mixture can be calculated, and is found to be, D $_{3m}$ = 1.588 * 10⁻⁵ m²/sec.

3.4.2 Diffusivity in liquids:

Diffusivity in liquid are exemplified by the values given in table ... Most of these values are nearer to 10^{-5} cm² / sec, and about ten thousand times shower than those in dilute gases. This characteristic of liquid diffusion often limits the overall rate of processes accruing in liquids (such as reaction between two components in liquids).

In chemistry, diffusivity limits the rate of acid-base reactions; in the chemical industry, diffusion is responsible for the rates of liquid-liquid extraction. Diffusion in liquids is important because it is slow.

Certain molecules diffuse as molecules, while others which are designated as electrolytes ionize in solutions and diffuse as ions. For example, sodium chloride (NaCl), diffuses in water as ions Na ⁺ and Cl⁻. Though each ions has a different mobility, the electrical neutrality of the solution indicates the ions must diffuse at the same rate; accordingly it is possible to speak of a diffusion coefficient for molecular electrolytes such as NaCl. However, if several ions are present, the diffusion rates of the individual cations and anions must be considered, and molecular diffusion coefficients have no meaning.

Diffusivity varies inversely with viscosity when the ratio of solute to solvent ratio exceeds five. In extremely high viscosity materials, diffusion becomes independent of viscosity.

3.4.3 Diffusivity in solids:

Typical values for diffusivity in solids are shown in table. One outstanding characteristic of these values is their small size, usually thousands of time less than those in a liquid, which are inturn 10,000 times less than those in a gas.

Diffusion plays a major role in catalysis and is important to the chemical engineer. For metallurgists, diffusion of atoms within the solids is of more importance.

3.5 Steady State Diffusion

In this section, steady-state molecular mass transfer through simple systems in which the concentration and molar flux are functions of a single space coordinate will be considered.

In a binary system, containing A and B, this molar flux in the direction of z, as given by Eqn (5) is [section 3.3.1]

$$N_{A} = -CD_{AB}\frac{dy_{A}}{dz} + y_{A}(N_{A} + N_{B}) - (1)$$

3.5.1 Diffusion through a stagnant gas film

The diffusivity or diffusion coefficient for a gas can be measured, experimentally using Arnold diffusion cell. This cell is illustrated schematically in figure.

The narrow tube of uniform cross section which is partially filled with pure liquid A, is maintained at a constant temperature and pressure. Gas B which flows across the open end of the tub, has a negligible solubility in liquid A, and is also chemically inert to A. (i.e. no reaction between A & B).

Component A vaporizes and diffuses into the gas phase; the rate of vaporization may be physically measured and may also be mathematically expressed interms of the molar flux.

Consider the control volume S Δ z, where S is the cross sectional area of the tube. Mass balance on A over this control volume for a steady-state operation yields

[Moles of A leaving at $z + \Delta z$] – [Moles of A entering at z] = 0.

(i.e.)
$$SN_A|_{z+\Delta z} - SN_A|_z = 0.$$
 ------(1)

Dividing through by the volume, S ΔZ , and evaluating in the limit as ΔZ approaches zero, we obtain the differential equation

$$\frac{dN_A}{dz} = 0 \qquad \dots \qquad (2)$$

This relation stipulates a constant molar flux of A throughout the gas phase from Z_1 to Z_2 .

A similar differential equation could also be written for component B as,

$$\frac{dN_B}{dZ} = 0,$$

and accordingly, the molar flux of B is also constant over the entire diffusion path from z_1 and z_2 .

Considering only at plane z_1 , and since the gas B is insoluble is liquid A, we realize that N_B , the net flux of B, is zero throughout the diffusion path; accordingly B is a stagnant gas.

From equation (1) (of section 3.5)

$$N_A = -CD_{AB}\frac{dy_A}{dz} + y_A(N_A + N_B)$$

Since N $_{\rm B} = 0$,

$$N_A = -CD_{AB}\frac{dy_A}{dz} + y_AN_A$$

Rearranging,

$$N_{A} = \frac{-CD_{AB}}{1-y_{A}} \frac{dy_{A}}{dz} \qquad -----(3)$$

This equation may be integrated between the two boundary conditions:

 $\begin{array}{ll} \mbox{at } z = z_1 & Y_A = Y_{A1} \\ \mbox{And} & \mbox{at } z = z_2 & Y_A = y_{A2} \end{array}$

Assuming the diffusivity is to be independent of concentration, and realizing that N_A is constant along the diffusion path, by integrating equation (3) we obtain

$$N_{A} \int_{Z_{1}}^{Z_{2}} dz = C D_{AB} \int_{y_{A1}}^{y_{A2}} \frac{-dy_{A}}{1 - y_{A}}$$

$$N_{A} = \frac{CD_{AB}}{Z_{2} - Z_{1}} \ln \left(\frac{1 - y_{A2}}{1 - y_{A1}} \right) -\dots -(4)$$

The log mean average concentration of component B is defined as

$$y_{B,Im} = \frac{y_{B2} - y_{B1}}{\ln \begin{pmatrix} y_{B2} \\ y_{B1} \end{pmatrix}}$$

Since $y_B = 1 - y_A$,

$$y_{B,Im} = \frac{(1 - y_{A2}) - (1 - y_{A1})}{\ln \begin{pmatrix} y_{A2} \\ y_{A1} \end{pmatrix}} = \frac{y_{A1} - y_{A2}}{\ln \begin{pmatrix} y_{A2} \\ y_{A1} \end{pmatrix}} \quad ----- (5)$$

Substituting from Eqn (5) in Eqn (4),

For an ideal gas $C = \frac{n}{V} = \frac{p}{RT}$, and

for mixture of ideal gases
$$y_A = \frac{p_A}{P}$$

Therefore, for an ideal gas mixture equation. (6) becomes

$$N_{A} = \frac{D_{AB}}{RT(z_{2} - z_{1})} \frac{(p_{A1} - p_{A2})}{p_{B,Im}}$$

This is the equation of molar flux for steady state diffusion of one gas through a second stagnant gas.

Many mass-transfer operations involve the diffusion of one gas component through another non-diffusing component; absorption and humidification are typical operations defined by these equation.

The concentration profile $(y_A vs. z)$ for this type of diffusion is shown in figure:

Oxygen is diffusing in a mixture of oxygen-nitrogen at 1 std atm, 25°C. Concentration of oxygen at planes 2 mm apart are 10 and 20 volume % respectively. Nitrogen is non-diffusing.

- (a) Derive the appropriate expression to calculate the flux oxygen. Define units of each term clearly.
- (b) Calculate the flux of oxygen. Diffusivity of oxygen in nitrogen = $1.89 \times 10^{-5} \text{ m}^2/\text{sec.}$

Solution:

Let us denote oxygen as A and nitrogen as B. Flux of A (i.e.) N _A is made up of two components, namely that resulting from the bulk motion of A (i.e.), Nx _A and that resulting from molecular diffusion J_A :

$$N_{A} = N x_{A} + J_{A}$$
 ------(1)

From Fick's law of diffusion,

$$J_A = -D_{AB} \frac{dC_A}{dz}$$
 (2)

Substituting this equation (1)

$$N_A = N x_A - D_{AB} \frac{d C_A}{d z} \qquad (3)$$

Since $N = N_A + N_B$ and $x_A = C_A / C$ equation (3) becomes

$$N_{A} = \left(N_{A} + N_{B}\right)\frac{C_{A}}{C} - D_{AB}\frac{dC_{A}}{dz}$$

Rearranging the terms and integrating between the planes between 1 and 2,

$$\int \frac{dz}{cD_{AB}} = -\int_{C_{A1}}^{C_{A2}} \frac{dC_A}{N_A C - C_A (N_A + N_B)} - \dots$$
(4)

Since B is non diffusing N $_{\rm B}$ = 0. Also, the total concentration C remains constant. Therefore, equation (4) becomes

$$\frac{z}{CD_{AB}} = -\int_{C_{A1}}^{C_{A2}} \frac{dC_A}{N_A C - N_A C_A}$$
$$= \frac{1}{N_A} \ln \frac{C - C_{A2}}{C - C_{A1}}$$

Therefore,

$$N_A = \frac{CD_{AB}}{z} \ln \frac{C - C_{A2}}{C - C_{A1}}$$
 ------(5)

Replacing concentration in terms of pressures using Ideal gas law, equation (5) becomes

$$N_{A} = \frac{D_{AB} P_{t}}{RTz} \ln \frac{P_{t} - P_{A2}}{P_{t} - P_{A1}}$$
 (6)

where

D_{AB} = molecular diffusivity of A in B

- P_T = total pressure of system
- R = universal gas constant
- T = temperature of system in absolute scale
- z = distance between two planes across the direction of diffusion
- P_{A1} = partial pressure of A at plane 1, and
- P_{A2} = partial pressure of A at plane 2

3.5.2 Psuedo steady state diffusion through a stagnant film:

In many mass transfer operations, one of the boundaries may move with time. If the length of the diffusion path changes a small amount over a long period of time, a pseudo steady state diffusion model may be used. When this condition exists, the equation of steady state diffusion through stagnant gas' can be used to find the flux.

If the difference in the level of liquid A over the time interval considered is only a small

fraction of the total diffusion path, and $t_0 - t$ is relatively long period of time, at any given instant in that period, the molar flux in the gas phase may be evaluated by

where z equals $z_2 - z_1$, the length of the diffusion path at time t.

The molar flux N_A is related to the amount of A leaving the liquid by

$$N_A = \frac{\rho_{A,L}}{M_A} \frac{dz}{dt} \qquad (2)$$

where $\frac{\rho_{A,L}}{M_A}$ is the molar density of A in the liquid phase

under Psuedo steady state conditions, equations (1) & (2) can be equated to give

Equation. (3) may be integrated from t = 0 to t and from $z = z_{t0}$ to $z = z_t$ as:

$$\int_{t=0}^{t} dt = \frac{\rho_{A,L} y_{B,Im} / M_A}{C D_{AB} (y_{A1} - y_{A2})} \int_{Z_{t0}}^{Z_t} z \, dz$$

yielding

This shall be rearranged to evaluate diffusivity D_{AB} as,

$$D_{AB} = \frac{\rho_{A,L} \, y_{B,Im}}{M_A \, C \, (y_{A1} - y_{A2}) \, t} \, \left(\frac{z_t^2 - z_{t0}^2}{2} \right)$$

3.5.3 Equimolar counter diffusion:

A physical situation which is encountered in the distillation of two constituents whose molar latent heats of vaporization are essentially equal, stipulates that the flux of one gaseous component is equal to but acting in the opposite direction from the other gaseous component; that is, $N_A = -N_B$.

The molar flux N_A, for a binary system at constant temperature and pressure is described by

or

with the substitution of N_B = - N_A , Equation (1) becomes,

$$N_A = -D_{AB} \frac{dC_A}{dz} \quad \dots \quad (2)$$

For steady state diffusion Equation. (2) may be integrated, using the boundary conditions:

at
$$z = z_1$$
 $C_A = C_{A1}$

and
$$z = z_2$$
 $C_A = C_{A2}$

Giving,

$$N_{A} \int_{Z_{1}}^{Z_{2}} dz = -D_{AB} \int_{C_{A1}}^{C_{A2}} dC_{A}$$

from which

$$N_A = \frac{D_{AB}}{z_2 - z_1} (C_{A1} - C_{A2})$$
 ------(3)

For ideal gases, $C_A = \frac{n_A}{V} = \frac{p_A}{RT}$. Therefore Equation. (3) becomes

$$N_{A} = \frac{D_{AB}}{RT(z_{2}-z_{1})} (P_{A1} - P_{A2}) - \dots (4)$$

This is the equation of molar flux for steady-state equimolar counter diffusion.

Concentration profile in these equimolar counter diffusion may be obtained from,

$$\frac{d}{dz}(N_A) = 0$$
 (Since N_A is constant over the diffusion path).

And from equation. (2)

$$N_A = -D_{AB} \frac{dC_A}{dz}.$$

Therefore

$$\frac{d}{dz}\left(-D_{AB}\frac{dC_{A}}{dz}\right) = 0$$

$$\frac{d^2 C_A}{dz^2} = 0$$

This equation may be solved using the boundary conditions to give

Equation, (5) indicates a linear concentration profile for equimolar counter diffusion.

For equimolar counter current diffusion:

$$N_{A} = \frac{D_{AB}}{RTz} \left(p_{A1} - p_{A2} \right) - \dots$$
 (1)

Diffusion in Liquids:

Equation derived for diffusion in gases equally applies to diffusion in liquids with some modifications. Mole fraction in liquid phases is normally written as 'x' (in gases as y). The concentration term 'C' is replaced by average molar density, $\left(\frac{\rho}{M}\right)_{av}$.

a) For steady – state diffusion of A through non diffusivity B:

$$N_{\rm A}$$
 = constant , $N_{\rm B}$ = 0

$$N_{A} = \frac{D_{AB}}{z x_{BM}} \left(\frac{\rho}{M}\right)_{av} \left(x_{A1} - x_{A2}\right)$$

where $Z = Z_2 - Z_1$, the length of diffusion path; and

$$X_{BM} = \frac{X_{B2} - X_{B1}}{\ln \begin{pmatrix} X_{B2} \\ X_{B1} \end{pmatrix}}$$

b) For steady – state equimolar counter diffusion :

$$N_A = -N_B = const$$

$$N_{A} = \frac{D_{AB}}{Z} (C_{A1} - C_{A2}) = \frac{D_{AB}}{Z} (\frac{\rho}{M})_{av} (x_{A1} - x_{A2})$$

Diffusion in solids

In certain unit operation of chemical engineering such as in drying or in absorption, mass transfer takes place between a solid and a fluid phase. If the transferred species is distributed uniformly in the solid phase and forms a homogeneous medium, the diffusion of the species in the solid phase is said to be structure independent. In this cases diffusivity or diffusion coefficient is direction – independent.

At steady state, and for mass diffusion which is independent of the solid matrix structure, the molar flux in the z direction is :

$$N_A = -D_{AB} \frac{dC_A}{dz} = \text{constant}$$
, as given by Fick's law.

Integrating the above equation,

$$N_A = \frac{D_{AB} \left(C_{A1} - C_{A2} \right)}{z}$$

which is similar to the expression obtained for diffusion in a stagnant fluid with no bulk motion (i.e. N = 0).

Diffusion in process solids:

In some chemical operations, such as heterogeneous catalysis, an important factor, affecting the rate of reaction is the diffusions of the gaseous component through a porous solid. The effective diffusivity in the solid is reduced below what it could be in a free fluid, for two reasons. First, the tortuous nature of the path increases the distance, which a molecule must travel to advance a given distance in the solid. Second, the free cross – sectional area is restricted. For many catalyst pellets, the effective diffusivity of a gaseous component is of the order of one tenth of its value in a free gas.

If the pressure is low enough and the pores are small enough, the gas molecules will collide with the walls more frequently than with each other. This is known as Knudsen flow or Knudsen diffusion. Upon hitting the wall, the molecules are momentarily absorbed and then given off in random directions. The gas flux is reduced by the wall collisions.

By use of the kinetic flux is the concentration gradient is independent of pressure ; whereas the proportionality constant for molecular diffusion in gases (i.e. Diffusivity) is inversely proportional to pressure.

Knudsen diffusion occurs when the size of the pore is of the order of the mean free path of the diffusing molecule.

3.6 Transient Diffusion/Unsteady state diffusion

Transient processes, in which the concentration at a given point varies with time, are referred to as unsteady state processes or time – dependent processes. This variation in concentration is associated with a variation in the mass flux.

These generally fall into two categories:

- i) the process which is in an unsteady state only during its initial startup, and
- ii) the process which is in a batch operation throughout its operation.

In unsteady state processes there are three variables-concentration, time,

and position. Therefore the diffusion process must be described by partial rather than ordinary differential equations.

Although the differential equations for unsteady state diffusion are easy to establish, most solutions to these equations have been limited to situations involving simple geometries and boundary conditions, and a constant diffusion coefficient.

Many solutions are for one-directional mass transfer as defined by Fick's second law of diffusion :

This partial differential equation describes a physical situation in which there is no bulk-motion contribution, and there is no chemical reaction. This situation is encountered when the diffusion takes place in solids, in stationary liquids, or in system having equimolar counter diffusion. The solution to Fick's second law usually has one of the two standard forms. It may appear in the form of a trigonometric series which converges for large values of time, or it may involve series of error functions or related integrals which are most suitable for numerical evaluation at small values of time. These solutions are commonly obtained by using the mathematical techniques of separation of variables or Laplace transforms.

Types of Solid Diffusion

The nature of solids and its interaction with the diffusing substance influence the rate of mass transfer. Different types of solid diffusion are discussed below.

Diffusion through polymers

Diffusion through polymeric membranes, e.g. gaseous separation through a membrane, mainly depends on the pressure gradient as the driving force. *Diffusion takes place from high pressure region to low pressure region*. A particular activation energy is needed for diffusion to take place and the temperature dependency of diffusivity is given by Arrhenius type relation,

$$D_{\rm A} = D_o \exp\left[\frac{-H_D}{RT}\right]$$

where H_D is the energy of activation and D_o is a constant. For simple gases, D_A is independent of concentration but for permanent gases, diffusivity is strongly
dependent on solute concentration in the solid. The diffusional flux is given by

$$V_{\rm A} = \frac{D_{\rm A} S_{\rm A} (p_{\rm A1} - p_{\rm A2})}{Z}$$

where

 V_A is the diffusional flux, cm³ · gas (STP)/cm²s

 $D_{\rm A}$ is the diffusivity of A, cm²/s

 p_A is the partial pressure of diffusing gas, cm Hg

 S_A is the solubility coefficient, cm³ · gas (STP)/cm³ solid · cm Hg

Z is the thickness of polymeric membrane, cm

Permeability can be defined as

$$P = D_A S_A$$

where P is the permeability, $cm^3 gas \cdot (STP)/cm^2 \cdot s$ (cm Hg/cm) The solubility is related to concentration in SI units as,

 $c_{\rm A}$ (kmol/m³ solid) = $Sp_{\rm A}$ = 22.414

and in CGS system as c_A (g mol/cm³ solid) = $Sp_A = 22414$

Diffusion through crystalline solids

Solute nature and crystalline structure are the important parameters in this type of diffusion. Some of the mechanisms followed for diffusion through crystal geometry are given below:

- Interstitial mechanism—Solute atoms diffuse from one interstitial site to the next in the crystal lattice.
- Vacancy mechanism—If lattice sites are vacant, an atom in an adjacent site may jump into the vacant site.
- Interstitialcy mechanism—A large atom occupying in an interstitial site pushes the neighbouring lattice into an interstitial position and moves into the vacancy produced.
- Crowded-ion mechanism—An extra atom in a chain of close-packed atoms can displace several atoms in the line from their equilibrium position.
- 5. Diffusion along grain boundaries—Diffusion takes place in crystal interfaces and dislocatic

Diffusion in porous solids

The solid may be porous in nature such as adsorbents or membrane and the diffusion takes place either by virtue of concentration gradient or by hydrodynamic flow behaviour because of pressure difference. In steady state diffusion of gases, there are two types of diffusive movement, depending on the ratio of pore diameter d, to the mean free path of the gas molecules, λ .

If the ratio $d/\lambda > 20$, molecular diffusion predominates

$$N_{\rm A} = \left(\frac{N_{\rm A}}{N_{\rm A} + N_{\rm B}}\right) \left(\frac{D_{\rm AB,eff} P_t}{RTZ}\right) \ln \left[\frac{\frac{N_{\rm A}}{N_{\rm A} + N_{\rm B}} - y_{\rm A2}}{\frac{N_{\rm A}}{N_{\rm A} + N_{\rm B}} - y_{\rm A1}}\right]$$
(2.62)

If $d/\lambda < 0.2$, the rate of diffusion is governed by the collisions of the gas molecules within the pore walls and follows Knudsen's law.

$$N_{\rm A} = \frac{D_{\rm K,A} \left(p_{\rm A1} - p_{\rm A2}\right)}{RTl}$$

where

 $D_{\rm K,A}$ is the Knudsen diffusivity, cm²/s

l is the length of the pore, cm

 p_A is the partial pressure of diffusing substance, cmHg

Knudsen diffusivity can be determined by using an empirical relation,

$$D_{\rm K,A} = \left(\frac{d}{3}\right) \left(\frac{8 g_c RT}{\pi M_A}\right)^{1/2}$$

2.5.2 Unsteady State Diffusion

Since solids are not readily transported, as fluids, unsteady state diffusional conditions arise more frequently in solids than in fluids. For unsteady state diffusion, Fick's second law is applied,

$$\frac{\partial C}{\partial t} = D_{AB} \left[\frac{\partial^2 C_A}{\partial x^2} + \frac{\partial^2 C_A}{\partial y^2} + \frac{\partial^2 C_A}{\partial z^2} \right]$$
(2.67)

Theories of mass transfer

Various theories have been used as models for explaining the turbulent mass transfer. These models can be used for predicting the mass transfer coefficients and they can be correlated with experimental data to obtain the design parameters of process equipments.

Film Theory

Consider turbulent flow of liquid over a solid surface and a simultaneous mass transfer is taking place. The film theory postulates that there is a stagnant film of thickness, Z_f adjacent to the interface, where the concentration difference is attributed to molecular diffusion as shown in Fig. 3.3. As the molecular diffusion is occurring only in Z_f , the flux equation can be written as

$$N_{\rm A} = k_C \left(C_{\rm A1} - C_{\rm A2} \right) = \left(\frac{D_{\rm AB}}{Z_f} \right) (C_{\rm A1} - C_{\rm A2}) \tag{3.21}$$

where $(C_{A1} - C_{A2})$ is the concentration difference. Hence, $k_C = (D_{AB}/Z_f)$, the mass transfer coefficient is proportional to $D_{AB}^{1.0}$. However, the J_D factor is given by,

$$J_D = \left(\frac{k_C}{V}\right) (N_{\rm Sc})^{2/3} = \left(\frac{k_C}{V}\right) \left(\frac{\mu}{\rho D_{\rm AB}}\right)^{2/3}$$
(3.22)

Hence, the film theory deviates from the actual turbulent mass transfer.



Penetration Theory

This theory explains the mass transfer at fluid surface and was proposed by Higbie. In many situations, the time of exposure for mass transfer is too short and hence, there may not be sufficient time for the steady state concentration gradient of film theory to develop. This theory has been described in Fig. 3.4. An eddy b, rising



from the turbulent liquid is exposed for a short time, θ at the interface for absorption. In this situation, the exposure time is assumed to be constant for all the eddies or particles of liquid.

Initially the eddy concentration is C_{A0} and when it comes to the surface, the interfacial concentration is C_{Ai} . Since the exposure time is less, molecules of solute from gas never reach the depth Z_b , which is nothing but the thickness of eddy. The liquid particle is subjected to unsteady state diffusion and hence Fick's second law is applicable, i.e.

$$\frac{\partial C_{\rm A}}{\partial \theta} = D_{\rm AB} \left[\frac{\partial^2 C_{\rm A}}{\partial Z^2} \right]$$

From the solute point of view, the depth Z_b is considered to be infinite. The boundary conditions are as follows:

$$C_{A} = C_{A0} \text{ at } \theta = 0 \text{ for all } Z$$

$$C_{A} = C_{Ai} \text{ at } Z = 0 \ \theta > 0$$

$$C_{A} = C_{A0} \text{ at } Z = \infty \text{ for all } \theta$$

By solving the above Eq. (3.23), the average flux can be obtained as described in falling film

Hence,

$$N_{A,av} = 2(C_{Ai} - C_{A0})\sqrt{\frac{D_{AB}}{\pi\theta}}$$
$$k_{L,av} = \sqrt{\frac{D_{AB}}{\pi\theta}}$$

Thus, in penetration theory k_L is proportional to $D_{AB}^{0.5}$. However, the exponent on D_{AB} varies from zero to 0.8 or 0.9.

Surface Renewal Theory

In reality, the time of exposure of all eddies as proposed in penetration theory is not constant. Hence, Danckwerts modified the penetration theory to account for varying lengths of time of exposure.

If S is the fractional rate of replacement of elements,

Then,
$$N_{A,av} = (C_{Ai} - C_{A0})\sqrt{D_{AB}S}$$

Hence, $k_{L,av}$ is proportional to $D_{AB}^{0.5}$ in this theory.

Combination of Film-Surface Renewal Theory

Film theory is meant for steady state diffusion where $k_L \propto D_{AB}$ and in surface renewal theory, $k_L \propto D_{AB}^{0.5}$. So k_L is proportional to D_{AB}^n with 'n' dependent upon circumstances. In this theory Dobbins replaced the third boundary condition of Eq. (3.23) by $C_A = C_{A0}$ at $Z = Z_b$, where Z_b is of finite depth. Finally he obtained

$$k_{\rm L,av} = \sqrt{D_{\rm AB}S} \operatorname{coth} \sqrt{\frac{SZ_b^2}{D_{\rm AB}}}$$

Surface-Stretch Theory

Lightfoot and his coworkers explained this theory where they found that the mass transfer at the interface varies with time periodically. When mass transfer is proceeding for a particular system the central portion of the drop is thoroughly turbulent and resistance to mass transfer resides in a surface layer with varying thickness and the drop is elongated as shown in Fig. 3.5. According to this theory,

$$k_{\mathrm{L,av}} = \frac{\left[(A/A_r) \sqrt{\frac{D_{\mathrm{AB}}}{\pi \theta_r}} \right]}{\sqrt{\int_{0}^{\theta/\theta r} (A/A_r)^2 d\theta}}$$

where A is time dependent interfacial surface, A_r is reference value of A, defined for every situation and θ_r is constant with dimensions of time or drop formation time.



SCHOOL OF BIO & CHEMICAL ENGINEERING

DEPARTMENT OF CHEMICAL ENGINEERING

UNIT – V – Transport Phenomena for Bioprocesses – SCHA1511

Modelling in a biological process

Model

Mathematical modeling and computer simulations can help us to;

- understand the nature and dynamics of biological processes
- to predict the future of the biological process
- to predict their interactions with the environment.
- What is a model?

- a model is an abstract representation of objects or processes that explains features of objects or processes.

- e.g. the letters A, C, G, and T are used as a model for DNA sequences.

Model Assignment is not Unique

Biological phenomena can be described in mathematical models. These models are not specific or unique to an organism or process. An organism can be studied with different experimental methods. A biological process can be described with different models. A model may be applied to different biological objects.

Properties of models

There is choice in selecting a model or an algorithm to describe a biological object. We may use different models but the modeling has to reflect essential properties of the system.

Different models may highlight different aspects of the same process or an organism.

System State

The state of a system is a snapshot of the system at a given time that contains enough information to predict the behavior of the system for all future time. Different models have different representations of the state. Each model defines what it means by the state of the system. Given the current state, the model predicts which state or states can occur next, thereby describing the change of state.

Steady State

Steady states, (stationary states or fixed points) – the values of all state variables remain constant in time. The steady state is actually an abstraction that is based on separation of time scales. Fast and slow processes are coupled in the biological world – -

Fast - formation and release of chemical bonds – nano secs.

Slow - growth of organisms - years.

Fast processes reach a quasi-steady state after a short period. Slow processes are mostly in the steady state or their change is negligible. Each steady state can be regarded as a quasi-steady state of a system that is in a larger non-stationary (steady) environment. Steady states point to typical behavioral modes of the system and hence the respective mathematical problems are easier to solve. Variables, Parameters, and Constants. All models have variables, parameters, and constants. A constant is a quantity with a fixed value, such as the natural number e or Avogadro's number. Parameters are quantities that are assigned a value, enzyme concentration – the value may change. Variables are quantities with a changeable value. State variables are a set of variables that describe the system behavior completely. They are independent of each other and each of them is necessary to define the system state.

For example, diameter d and volume V of a sphere obey the relation V = $\pi d3/6$.

• Volume of a sphere V = $\pi d3/6$

• π and 6 are constants and V and d were the variables, but only one of them is a state variable, since the mentioned relation uniquely determines the other one. Whether a quantity is a variable or a parameter depends on the model. The enzyme concentration is frequently considered a parameter in biochemical reaction kinetics. no longer valid if, in a larger model, the enzyme concentration may change due to gene expression or protein degradation.

Model behaviour

Model behavior is determined by (1) influences from the environment (input) and (2) processes within the system. Further, the system structure, (i. e., the relation among variables, parameters, and constants) determines how the external inputs are processed and how the internal processes are controlled.

Process classification

- Reversible process can proceed in forward or backward direction.
- Irreversible process can proceed in only one direction
- Periodicity at specific time intervals the state of the process may change.
- Deterministic the future state of the process may be determined

by the current state.

• Stochastic – future state cannot be determined – only a probability

can be predicted.

- Continuous the values of the state are continuous.
- Discrete the values of the state are discrete (not continuous).

Advantages of Computational Modeling

• Modeling gives conceptual clarification – makes things understandable – Eg. AGTC for nucleotides.

• Modeling also highlights gaps in knowledge or understanding – if a model fails to mimic the real experiment then there is a gap.

• Modeling provides independence from the modeled object. Time and space may be stretched or compressed ad libitum.

• Modeling is cheap compared to experiments. Models do no harm on animals or plants and help to reduce them in experiments.

• They do not pollute the environment. Models do not interact with the environment or with the modeled system.

• Modeling can assist experimentation. With an adequate model one may test different possibilities that are not available in experiment.

• One may follow time courses of compounds that cannot be measured in an experiment. Eg. Aging process

• One may impose perturbations that are not feasible in the real system. Eg. Effect of a toxin.

• One may cause precise perturbations without directly changing other system components, which is usually impossible in real systems.

- Model simulations can be repeated for many different conditions.
- Model results can often be presented in precise mathematical terms that allow for generalization.
- Graphical representation and visualization make it easier to understand the system.
- Finally, modeling allows for making well-founded and testable predictions.

Model Development – Modeling Workflow

1. Formulation of the problem:

- which questions shall be answered with the model
- clear statement about the background, problem, and hypotheses
- 2. Verification of available information:

- the existing data about the structure of the system has to be collected and checked.

3. Selection of model structure:

- determine the general type of the model like 1) microscopic or macroscopic, 2) deterministic or stochastic approach, 3) discrete or continuous variables, 4) steady-state, temporal, or spatiotemporal description. Find variables for external influence, internal structure.

4. Establishing a simple model:

- model can be in words, scheme in mathematical formulation.

5. Sensitivity analysis:

- mathematical simulation may be highly sensitive to parameter changes. Verify the parameter choice.

6. Experimental tests of the model predictions:

7. Stating the agreements and divergences between experimental and modeling results:

- whether the model results agree with the experimental behavior

- if results do not agree, check for false assumptions, over simplification, wrong model structure, inadequate experimental design, or other inadequately represented factors.

8. Iterative refinement of model:

- usually initial models may not be correct. Refine continuously till the model adequately represents the biological system.

Steady and Pseudo steady state approximation

When a reaction mechanism has several steps of comparable rates, the rate-determining step is often not obvious. However, there is an intermediate in some of the steps. An intermediate is a species that is neither one of the reactants, nor one of the products. The steady-state approximation is a method used to derive a rate law. The method is based on the assumption that one intermediate in the reaction mechanism is consumed as quickly as it is generated. Its concentration remains the same in a duration of the reaction.

Definition: Intermediates

An intermediate is a species that is neither one of the reactants, nor one of the products. It transiently exists during the course of the reaction. When a reaction involves one or more intermediates, the concentration of one of the intermediates remains constant at some stage of the reaction. Thus, the system has reached a steady-state. The concentration of one of the intermediates, [Int], varies with time as shown in Figure 4.12.1. At the start and end of the reaction, [Int] does vary with time.

d[Int]/dt=0

Example: when an intermediate can be approximated as a steady-state.

When a reaction mechanism has several steps with comparable rates, the rate-determining step is not obvious. However, there is an intermediate in some of the steps. The steady-state approximation implies that you select an intermediate in the reaction mechanism, and calculate its concentration by assuming that it is consumed as quickly as it is generated. In the following, an example is given to show how the steady-state approximation method work.

Michael Menton Kinetics

All these reactions involve a substrate S reacting with an enzyme E to form a complex ES which then in turn is converted into product P and the enzyme:

In this scheme there are two fundamental different reactions. The first reaction depicted with the double arrow is a reversible reaction reflecting the reversible binding and unbinding of the enzyme and the substrate. The second reaction is an irreversible reaction in which the enzyme-

substratecomplexisirreversiblyconverted into product and enzyme symbolized by the single arrow. The rate of a reaction is proportional to the product of the concentrations of the reactants. The kinetics of the chemical equations above is described by the following set of coupled differential equations:

In this case the systems can also be solved analytically. Figure 1 shows an example of the time dependence of the chemical components for $k_1[S_o] \approx k_{-1} \gg k_2$. This is often the regime of biological relevance since the substrate-enzyme binding occurs at much faster time scales than the turnover into product. The thermodynamic equilibriumor steady state $(t \rightarrow \infty)$ of this system would be [S] = [ES] = 0; $[E] = [E_o]$; [P] =

 $[S_o]. However, the relevant time-scale to consider is the time range in which [ES] and [E] are$

$$\frac{d[S]}{dt} = -k[E][S] + k[ES] \\ \frac{d[E]}{d[E]} = -k[E][S] + (k + k + k) \\ d[ES] = -k[E][S] - (k + k + k) \\ d[ES] = k[E][S] - (k + k + k) \\ dt = 1 + k + k \\ dt = 1 + k \\ dt = 1 + k + k \\ dt = 1 + k \\ dt$$

Note that k_1 and k_2 have different units, 1/(Ms) and 1/srespectively. The turnover rate $v \square$ is defined as the increase (or decrease) in product over time, which is directly proportional to the concentration of enzyme-substrate complex [ES]. For the analysis below we will assume initial conditions: $[S]_{t=0}=S_0$; $[E]_{t=0}=E_0$; $[ES]_{t=0}=0$; $[P]_{t=0}=0$.

Since the enzyme is a catalyst that facilitates the reaction but does not react itself,

thetotalconcentration of enzyme(free + bound) should be constant:

$$E_{o} = [E] + [ES]$$
 [I.3]

Using this conservation law the four differential equations [I.2] reduce to three coupled ordinary differential equations:

with the initial conditions [S]_{t=0} = S_o, [ES]_{t=0} = 0, and [P]_{t=0} = 0. Matlab code 1 solvestheseequationsandcalculatesthetimedependenceoftheconcentrations[S],[ES]and
[P] as a function of the initial concentrations [S_o] and [E_o] and the rate constants k₁, k₋₁, and k₂.

Ultracentrifuge

Ultracentrifugation has decisively advanced the detailed biochemical analysis of subcellular structures and isolated biomolecules. Preparative ultracentrifugation can be operated at relative centrifugal fields of up to 900 000×g. In order to minimise excessive rotor temperatures generated by frictional resistance between the spinning rotor and air, the rotor chamber is sealed, evacuated and refrigerated. Depending on the type, age and condition of a particular ultracentrifuge, cooling to the required running temperature and the generation of a stable vacuum might take a considerable amount of time. To avoid delays during biochemical procedures involving ultracentrifugation, the cooling and evacuation system of older centrifuge models should be switched on at least an hour prior to the centrifugation run. In contrast, modern ultracentrifuges can be started even without a fully established vacuum and will proceed in the evacuation of the rotor chamber during the initial acceleration process. For safety reasons, heavy armour plating encapsulates the ultracentrifuge to prevent injury to the user in case of uncontrolled rotor movements or dangerous vibrations. A centrifugation run cannot be initiated without proper closing of the chamber system. To prevent unfavourable fluctuations in chamber temperature, excessive vibrations or operation of rotors above their maximum rated speed, newer models of ultracentrifuges contain sophisticated temperature regulation systems, flexible drive shafts and an over-speed control device. Although slight rotor imbalances can be absorbed by modern ultracentrifuges, a more severe misbalance of tubes will cause the centrifuge to switch off automatically. This is especially true for swinging-bucket rotors. The many safety features

incorporated into modern ultracentrifuges make them a robust piece of equipment that tolerates a certain degree of misuse by an inexperienced operator. In contrast to preparative ultracentrifuges, analytical ultracentrifuges contain a solid rotor that incorporates one counterbalancing cell and typically either three or seven analytical cells. A specialised optical system enables the sedimenting material to be observed throughout the duration of a centrifuge run. Using either an absorption optical system (based on ultraviolet/visible light absorption; or a Rayleigh interference optical system (based on light refraction, or a combination of both, concentration distributions of macromolecules in solution can berecorded at any time during ultracentrifugation. From these records, information about the purity/heterogeneity, sedimentation coefficient distribution, average molar mass and molar mass distributions, and ligand interaction information can be obtained.

Types of Rotor

To illustrate the difference in design of fixed-angle rotor, vertical tube rotors and swinging-bucket rotors ,outlines cross-sectional diagrams of these three main types of rotor. Companies usually name rotors according to their design type, the maximum allowable speed and sometimes the material composition. Depending Centrifugal field Centrifugal field Centrifugal field Axis of rotor Axis of rotor Axis of rotor (a) (b) (c) Tube angle 14°-40° rmin ron the use in a simple low-speed centrifuge, a high-speed centrifuge or an ultracentrifuge, different centrifugal forces are encountered by a spinning rotor. Accordingly, different types of rotors are made from different materials. Low-speed rotors are usually made of steel or brass, while high-speed rotors consist of aluminium, titanium or fibre-reinforced composites. The exterior of specific rotors might be finished with protective paints. For example, rotors for ultracentrifugation made out of titanium alloy are covered with a polyurethane layer. Aluminium rotors are protected from corrosion by a tough, electrochemically formed layer of aluminium oxide. In order to avoid damaging these protective layers, care should be taken during rotor handling. Fixed-angle rotors are an ideal tool for pelleting during the differential separation of biological particles where sedimentation rates differ significantly, for example when separating nuclei, mitochondria and microsomes. In addition, isopycnic ('matching density') banding – where the density of the substance matches that of the gradient at that radial position – may also be routinely performed with fixed-angle rotors. For isopycnic separation, centrifugation is continued until the biological particles of interest have reached their isopycnic position in a gradient. This means that the particle has reached a position

where the sedimentation rate is zero because the density of the biological particle and the surrounding medium are equal. Centrifugation tubes are held at a fixed angle of between 14° and 40° to the vertical in this class of rotor. Particles move radially outwards and since the centrifugal fi eld is exerted at an angle, they only have to travel a short distance until they reach their isopycnic position in a gradient using an isodensity technique or before colliding with the outer wall of the centrifuge tube using a differential centrifugation method. Vertical rotors may be divided into true vertical rotors and near-vertical rotors. Sealed centrifuge tubes are held parallel to the axis of rotation in vertical rotors and are restrained in the rotor cavities by screws, special washers and plugs. Since samples are not separated down the length of the centrifuge tube, but across the diameter of the tube, isopycnic separation time is significantly shorter as compared to swingingbucket rotors. In contrast to fixed-angle rotors, near-vertical rotors exhibit a reduced tube angle of 7° to 10° and also employ quick-seal tubes. The reduced angle results in much shorter run times as compared to fi xed-angle rotors. Near-vertical rotors are useful for gradient centrifugation of biological elements that do not properly participate in conventional gradients. Hinge pins or a crossbar is used to attach rotor buckets in swinging-bucket rotors. They are loaded in a vertical position and during the initial acceleration phase, the rotor buckets swing out horizontally and then position themselves at the rotor body for support. To illustrate the separation of particles in the three main types of rotors, which outlines the path of biological samples during the initial acceleration stage, the main centrifugal separation phase, de-acceleration and the final harvesting of separated particles in the rotor atrest. In the case of isopycnic centrifugation in a fixed-angle rotor, the centrifuge tubes are gradually filled with a suitable gradient, the sample carefully loaded on top of this solution and then the tubes placed at a specific fixed-angle into the rotor cavities. During rotor acceleration, the sample solution and the gradient undergo reorientation in the centrifugal field, followed by theseparation of particles with different sedimentation properties. The gradient returns to its original position during the de-acceleration phase and separated particle bands can be taken from the tubes once the rotor is at rest. In analogy, similar reorientation of gradients and banding of particles occurs in a vertical rotor system.

Care and Maintenance of Centrifuges

Corrosion and degradation due to biological buffer systems used within rotors or contamination of the interior or exterior of the centrifuge via spillage may seriously affect the lifetime of this equipment. Another important point is the proper balancing of centrifuge tubes. This is not only important with respect to safety, as outlined below, but might also cause vibration-induced damage to the rotor itself and the drive shaft of the centrifuge. Thus, proper handling and care, as well as regular maintenance of both centrifuges and rotors, is an important part of keeping this biochemical method available in the laboratory. In order to avoid damaging the protective layers of rotors, such as polyurethane paint or aluminium oxide, care should be taken in the cleaning of the rotor exterior. Coarse brushes that may scratch the finish should not be used and only non-corrosive detergents employed. Corrosion may be triggered by long-term exposure of rotors to alkaline solutions, acidic buffers, aggressive detergents or salt. Thus, rotors should be thoroughly washed with distilled or deionised water after every run. For overnight storage, rotors should be first left upside down to drain excess liquid and then positioned in a safe and dry place.

To avoid damage to the hinge pins of swinging-bucket rotors, they should be dried with tissue paper following removal of biological buffers and washing with water. Centrifuge rotors are often not properly stored in a clean environment; this can quickly lead to the destruction of the protective rotor coating and should thus be avoided. It is advisable to keep rotors in a special clean room, physically separated from the actual centrifugation facility, with dedicated places for individual types of rotors. Some researchers might prefer to pre-cool their rotors prior to centrifugation by transferring them to a cold room. Although this is an acceptable practice and might keep proteolytic degradation to a minimum, rotors should not undergo long term storage in a wet and cold environment. Regular maintenance of rotors and centrifuges by engineers is important for ensuring the safe operation of a centralised centrifuge, it is essential that all users of core centrifuge equipment participate in proper book-keeping. Accurate record-keeping of run times and centrifugal speeds is important, since cyclic acceleration and deceleration of rotors may lead to metal fatigue.

Separation of DNA Components

A recent application of ultracentrifugation is in the genome-wide identification of gene regulatory regions, i.e. the open regions of DNA not protected by nucleosomes at that point in time. Intact nuclei are incubated with limiting amounts of DNase I, which is able to enter the nuclei and digest accessible DNA from chromatin. The digested DNA is then recovered and applied to a step gradient typically made with 10-400/o sucrose (400/0 at the bottom of the tube, rising to 100/0 at the top), and subjected to 24 hours at 90 000xg (at 25 °C). Alternatively a 'sucrose cushion' can be used that

is simply a fixed concentration of sucrose; typically 90/o. The gentle separation of DNA fragments allows efficient molecular cloning of the DNA fragments that are then sequenced using massively parallel sequencing.

ANALYTICAL ULTRACENTRIFUGATION

Analytical ultracentrifuges are high-speed ultracentrifuges with optical system(s) for recording the sedimentation process. As biological macromolecules exhibit random thermal motion, their relative uniform distribution in an aqueous environment is not significantly affected by the Earth's gravitational field. Isolated bio-molecules in solution only exhibit distinguishable sedimentation when they undergo immense accelerations, e.g. in an ultra centrifugal field. A typical analytical ultracentrifuge can generate a centrifugal field of up to 200 000xg in its analytical cell. Within these extremely high gravitational fields, the ultracentrifuge cell has to allow light passage through the biological particles for proper measurement of the concentration distribution. The schematic diagram in Figure 12.8 outlines one of the two principal optical systems for a modern analytical ultracentrifuge. The availability of high-intensity xenon flash lamps and the advance in instrumental sensitivity and wavelength range has made the measurement of highly dilute protein samples below 230 nm possible. Analytical ultracentrifuges such as the Beckman Optima XL-A allow the use of wavelengths between 190 nm and 800 nm. Sedimentation of isolated proteins or nucleic acids can be useful in the determination of the molecular mass, purity and shape of these biomolecules. A second optical system (not shown) is the Rayleigh interference optical system, which detects the distribution of proteins or nucleic acids - or other macromolecules such as polysaccharides, glycol proteins and synthetic macromolecules - based on their different refractive index compared to the solvent they are dissolved in. The Beckman Optima XL-I, for example, has both optical systems. These two different optical systems can be applied individually, or simultaneously, which can be helpful for looking at interactions involving biomolecules with ligands. Other less common optical systems are based on fluorescence or refractive gradient "Schlieren" optics.