Lecture Notes for CHE F414 : Transport Phenomena

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Introduction

This series of lecture notes will cover the three aspects of transport processes related to chemical engineering : momentum transport, energy transport and mass transport. As we proceed, we will draw analogies between the concepts and equations of these three types of transport and use them to solve relevant problems in chemical engineering.

The typical kind of problems involved in this subject would be analysing the transport processes of a fluid in a given domain of space. The best way to deal with these problems is to think of what fluid properties we want to track in that domain of space. For most chemical engineering problems, knowing the variation of fluid velocity, temperature and concentrations would suffice. We hence define a "field" over our domain of interest for each of these quantities. For temperature and concentrations, we can define a scalar field, while for velocities, we define a vector field. We can then use certain assumptions we make about the fluid flow and the domain of interest as well as a few physical laws to solve for these fields.

When describing transport, we can talk about fluids at three different scales. At the macroscopic level, we see how physical quantities vary with a bulk of the fluid. At this scale, we can abstract out most of the details between interactions of fluid molecules or fluid elements. At the microscopic level, we divide the bulk fluid into differential "fluid elements" and write down equations that describe their motion. At these two levels, we maintain a "continuum approximation", whereby we assume that the fluid or material is present at every point in space within the domain of interest. If we dig a little deeper and think about the fundamental mechanisms of transport in terms of molecular forces and properties, we get to the last scale at which we think about problems.

Chapter 1

Transport Mechanisms

1.1 Viscosity and Demonstrating Momentum Transport

Viscosity is a measure of a fluid's tendency to resist flow. Generally we represent the viscosity of a fluid by μ.

Before describing the properties of viscosity and how it changes, let us observe qualitatively how a viscous fluid behaves when we try to make it flow under some forces.

Given below is a simple, illustrative situation:

(a)   (b)   (c)

$t \leq 0$ $t = \delta$ $t \gg 0$
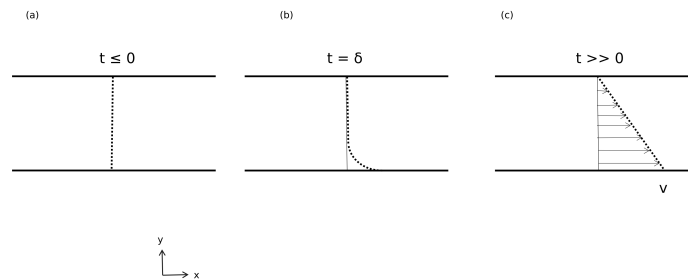
V

y

x

Figure 1.1: Fluid between 2 plates

- Consider two parallel plates : one placed at y = 0 and the other placed at y = Y as shown in figure 1.1, with a static fluid between them. Here we assume these plates are basically infinitely long and wide so that the fluid doesn't move. Figure 1.1(a) shows how the fluid velocity is 0 at every point between the two plates.

- Now, let us see what happens when we begin to translate the bottom plate to the right. Assuming there is no slip between the fluid and the plate, i.e. that the fluid that comes into contact with the solid is "stuck" to it. At the molecular scale, this is because we consider adhesive forces of attraction between molecules of the fluid and the solid are stronger than the cohesive forces of attraction among the molecules of the fluid themselves. So when we move the bottom plate, the molecules in contact with it start to move along. Figure 1.1(b) describes a snapshot of the system where the molecules "stuck" to the plate have just started to move but the molecules above them haven't been impacted yet.

- Over time, the fluid layers begin to pull each other and due to this, momentum gets imparted along the y direction. Figure 1.1(c) showcases the steady-state velocity profile of the fluid. Again, at the top plate the fluid doesn't move since the molecules are assumed to be "stuck" to the plate.

We began our observation of the transport of momentum by seeing how the fluid molecules in contact with the lower plate are dragged along. But it is important to note that the plate is also being dragged by the fluid! So we have to apply some force F to keep the plate going. How much does the fluid drag the plate?

$$\frac{F}{A} = \mu \frac{V}{Y}$$

This can be extended to looking at the force per unit area that each differential "slice" of fluid experiences:

$$\boxed{\tau_{yx} = -\mu \frac{dv_x}{dy}} \tag{1.1}$$

This is a very important equation and is referred to as Newton's Law of Viscosity. Some key points to note about Newton's Law of Viscosity:

- This equation showcases the transport of the x component of momentum in the y direction.

- $\tau_{xy} = F/A$ here refers to the force in x direction per unit area perpendicular to y direction. This quantity is the flux of x-component of momentum in the y direction.

- The law applies to other directions as well. If we consider a pair of **unequal** directions i, j, we can generalise this and state that

$$\tau_{ij} = -\mu \frac{dv_j}{di}$$

.

- If i = j, then we get (for example i = j = x)

$$\tau_{xx} = -2\mu \frac{dv_x}{dx}$$

.

- Here we consider μ to be invariant of the directions (we don't say μ_{xy} etc.). This makes an inherent assumption about the isotropy of the fluid, i.e. that the properties of the fluid don't vary in different directions. This is not necessarily true in certain complex fluids and polymer solutions.

Note that it's very easy to see how τ refers to "momentum flux" by just looking at dimensions. Force is (mass).(acceleration) = (mass).(velocity/time) = (momentum/-time) or rate of momentum. Now Force/Area is just flux of momentum, simple!

It is very important to remember that τ_{yx} is the flux of "x-momentum in y direction". It is easy to flip the order and make a mistake, so be careful.

Some more points on viscosity

- The dimensions of μ is (pressure).(time) and hence the SI unit is pascal-second or (Pa)(s). However a more convenient unit for engineering problems is centipoise (cP). Keep in mind that $1cP = 10^{-3}Pa.s$. Water has a viscosity of about 1 cP at room temperature.

- At low densities

    - **Gases:** Viscosity increases with temperature

    - **Liquids:** Viscosity decreases with temperature

- Kinematic viscosity can be defined as

$$\nu = \frac{\mu}{\rho}$$

- A useful quantity that describes the flow properties of a fluid is the Reynolds' number (Re). It is given by :

$$Re = \frac{\rho v d}{\mu}$$

where v is a characteristic velocity of the system and d is a characteristic length. It represents the ratio of inertial forces to viscous forces in a fluid system.

1.2 Mechanisms of Momentum Transport

1.2.1 Vectors and Tensors in Transport

Some important notation:

- **v** is the velocity vector.

- v_x is the x component of the velocity vector which is a function: $v_x(x,y,z,t)$.

- The unit vectors are denoted by δ_x, δ_y, δ_z in x, y, z directions.

- Tensors are multilinear objects relating vectors. In the case of fluids, we are mainly concerned with "order 2" tensors, which can be depicted similar to matrices. For example, τ is an order two tensor whose components are τ_{ij}.

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

- This is a 9-component tensor. The diagonal components represent normal stresses while other terms are shear stresses.

- We can also consider one component out of our tensors: which then becomes a vector. For example if we take the x component of τ, we have τ_x which is a vector.

1.2.2   Molecular Momentum Transport

Molecular transport of momentum is the extent of momentum transport that can be attributed to molecular forces. In figure 2, we take a differential fluid element and observe the forces. First let us only consider forces acting in the x-direction, for simplicity. For this, we observe a plane perpendicular to the x-axis (or parallel to the yz plane). For this plane there are 2 forces :

- Viscous force τ_x which has three components.

- Pressure force $P\delta x$. Note again that δ_x is the x-direction unit vector.
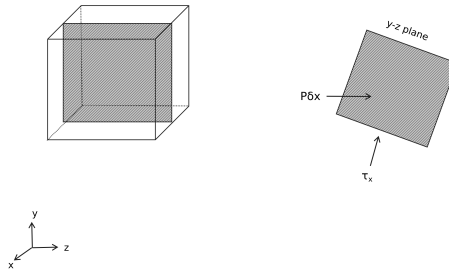

Figure 1.2: Forces on a fluid element

In the absence of a velocity gradient, there are no viscous forces since fluid elements move together but pressure forces still act.

Hence, there are 6 forces tugging this fluid element : 3 pressure forces $P\delta x, P\delta y, P\delta z$ and 3 viscous forces τ_x, τ_y, τ_z.

Now, we can define a **molecular momentum flux** (π) which gives us the flux of momentum due to molecular forces. We need it to incorporate the pressure term and the viscous term. As described in Figure 2, let us only consider this molecular momentum flux across a plane perpendicular to the x axis.

The viscous terms are easy to incorporate. π_{xx} would have the term τ_{xx}, π_{xy} would incorporate τ_{xy} and so on. The pressure term meanwhile only has one direction (x), so we expect it to appear only in the π_{xx} expression.

In summary :

$$\pi_{xx} = P + \tau_{xx}$$

$$\pi_{xy} = \tau_{xy}$$

$$\pi_{xz} = \tau_{xz}$$

Similar expressions can be written for π_y and π_z. For π_y the pressure term will appear in π_{yy} only and for π_z it'll appear only in π_{zz}.

If we wanted to condense our expression for π into one terse statement, we can write it as such :

$$\boxed{\pi_{ij} = P\delta_{ij} + \tau_{ij}} \tag{1.2}$$

Here δ_{ij} is the Kronecker delta function (which has a value of 1 when i = j and 0 otherwise). π_{ij} **is the flux of j-momentum in the i direction, from a region of less i to greater i.** π is again a tensor with the diagonal terms being normal stresses and other components being shear stresses.

1.2.3 Convective Momentum Transport

Apart from molecular forces, momentum can also be transported by bulk flow of fluid. This is called "convective momentum transport".

In figure 3, we see the same fluid element again, but this time let us only consider the convective terms. The volume rate of fluid flow across the shaded area is v_x. And it carries a momentum vector ρ **v** (here we look at momentum per unit volume). Hence the momentum flux is simply $v_x\rho$ **v**. This quantity is the convective momentum flux across a plane perpendicular to the x-axis.

The tensor for convective momentum transport can be represented as ρ **v v**. As in the case of molecular momentum flux tensor, this is also a 9-component tensor.

Combined Momentum Flux

To denote the total momentum flux experienced by a fluid in various directions, we use the tensor ϕ. It is the sum of molecular and convective momentum fluxes.
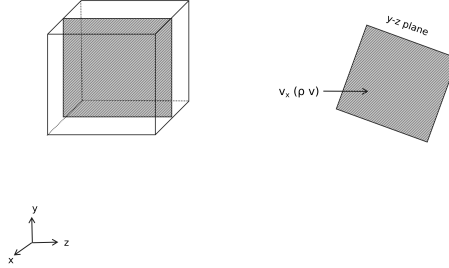
Figure 1.3: Convective Momentum Transport

$$\phi = \pi + \rho \mathbf{v} \, \mathbf{v}$$
(1.3)

Consider some example components of this tensor:

$$\phi_{zz} = P + \tau_{zz} + \rho v_z v_z$$

$$\phi_{xy} = \tau_{xy} + \rho v_x v_y$$

Questions

1. Consider a set of vectors v_i, where all the vectors are orthogonal (perpendicular) to each other. We want to develop a terse notation to show this orthogonality. Which of these are suitable?

   (a) $v_i \cdot v_j = |v|^2$
   (b) $v_i \cdot v_j = |v|^2 \delta_{ij}$
   (c) $v_i - v_j = (\delta_x - \delta_y)(|v_i| - |v_j|)$
   (d) $v_i + v_j = (\delta_x + \delta_y)(|v_i| + |v_j|)$

2. Two infinite parallel plates, separated by 1m have a viscous static fluid of viscosity 1 cP between them. The top plate is translated to the left with a velocity of 5 ms^{-1} and the bottom plate is translated to the right by 6 ms^{-1}. After reaching steady-state, what is the velocity of a fluid element half-way between the plates? Is that fluid element moving to the right or left?

3. A boat with sophisticated measurement machinery is going around a lake on a windy day and measuring stresses. The velocity of the lakewater at a point (x, y)

is given by $v_x(x,y), v_y(x,y)$, where $v_x(x,y) = Ae^{-(x+y)}$, $v_y(x,y) = B\frac{x+y}{xy}$ Write the components of the viscous stress tensor for this system.

4. Verify that the per-volume momentum $\rho\,\mathbf{v}$ when multiplied by velocity $\mathbf{v}$ does in fact give a momentum flux quantity.

1.3 Thermal Conductivity and Demonstrating Energy Transport

In a similar manner to how we saw the qualitative behaviour of a viscous fluid between two solid plates, we shall demonstrate the behaviour of thermal conductivity of a solid slab between two plates.
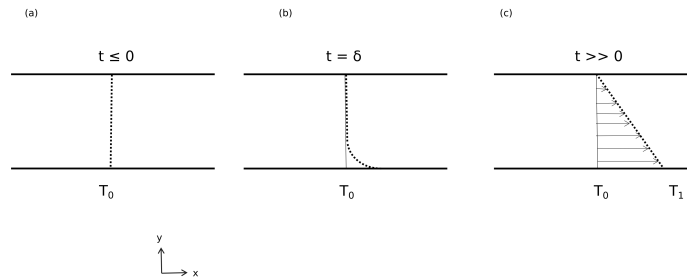

Figure 1.4: Solid slab of conducting material between 2 plates

- Consider two parallel plates : one placed at y = 0 and the other placed at y = Y as shown in figure 1.4, with a conducting solid between them. Here we assume these plates are basically infinitely long and wide. The system is at equilibrium with no heat sources anywhere. Figure 1.4(a) shows how the temperature is uniform at T_0 every point between the two plates.

- Now, let us see what happens when we add a heat bath to the lower plate so that its temperature is kept at a slightly higher temperature T_1. If the temperature of the lower plate is uniformly at a temperature T_1 and is in contact with the solid material, two phenomena could occur to get energy across to atoms in the solid:

    - Either free electrons in the solid start to move quickly across it and hence transfer thermal energy

    - The periodic vibrations of atoms in the solid move across (phonon transport)
    .

- Figure 1.4(b) describes a snapshot of the system where some of the thermal energy has started to go across to the interface atoms of the slab but most of it is still yet unaffected.

- Note that the top plate is still exposed to the environment, which is assumed to be at the temperature T_0. Over time, the solid atoms begin to transmit heat across by the two mechanisms mentioned above and energy gets imparted along the y direction. Figure 1.4(c) showcases the steady-state temperature profile of the slab.

In the case of momentum transport, we computed the force needed to keep the lower plate moving at a velocity v. Here, the lower plate keeps transmitting its heat energy off to the slab. So how much heat does the heat bath need to supply to the lower plate to keep its temperature constant at T_1?

$$\frac{Q}{A} = k\frac{\Delta T}{Y}$$

It's a very similar expression to our initial expression for the force on a viscous liquid. This can similarly be extended to looking at the heat flux across every differential slice of the solid slab and hence we get the equation :

$$\boxed{q_y = -k\frac{dT}{dy}} \tag{1.4}$$

This is called **Fourier's Law of Heat Conduction**.
Some points to note :

- Here, k is the thermal conductivity. It is a material property of the slab that describes the rate of heat conduction across it.

- Unlike fluid velocity, which is a vector, temperature is a scalar quantity. Similarly, in momentum transport, τ was a tensor. Here q is a vector with components q_x, q_y, q_z in directions perpendicular to the x, y and z axes. The multidimensional equivalent of Fourier's law is:

$$q = -k\nabla T$$

- We have again made an implicit assumption that the thermal conductivity of the material is isotropic and that k is the same in all directions. In the case of fibrous materials and laminates, we can use the following equation :

$$q = -\vec{\kappa}.\nabla T$$

where $\vec{\kappa}$ is a thermal conductivity tensor.

Some more points on thermal conductivity

- The thermal diffusivity of a system (α) is the ratio of heat conducted to heat stored. It is given by the expression

$$\alpha = \frac{k}{\rho C_p}$$

  where C_p is the heat capacity of the material

- There are two useful dimensionless constants in energy transport. The Prandtl number (Pr) given by :

$$Pr = \frac{C_p \mu}{k}$$

  and the Peclet number (Pe) given by

$$Pe = RePr = \frac{dv}{\alpha}$$

.

1.4 Mechanisms of Energy Transport

There are three primary methods for energy transport that we are concerned with : *Molecular Energy Transport* (which we have discussed thus far in the form of heat conduction), *Convective energy transport* and *Diffusive energy transport*.

1.4.1 Convective energy transport

Convective energy transport is the energy transported by bulk movement of the fluid.

Consider a differential fluid element. The convective energy transport can be represented by $q^{(c)}$. It is again a vector with three components. Let the x-component be $q_x^{(c)}$. Here the surface of area dS is in a direction perpendicular to the x-axis as indicated in figure 1.5. The volume rate of flow across this surface is $v_x dS$. Now to get the total energy passing through this differential element, we need the energy per unit volume of the fluid flowing through, which is the sum of the kinetic energy per unit volume and the internal energy per unit volume.

$$q_x^{(c)} = (\frac{1}{2}\rho v^2 + \rho U)v_x$$

Where, $v^2 = v_x^2 + v_y^2 + v_z^2$. Representing this equation in general for the overall vector, we get:

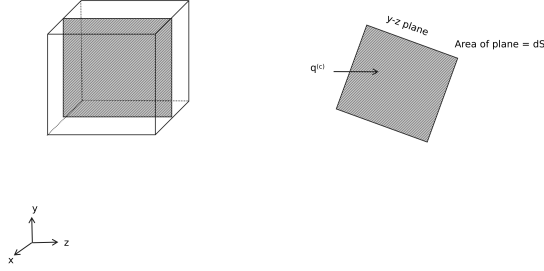$$\boxed{q^{(c)} = (\frac{1}{2}\rho v^2 + \rho U).\vec{v}} \qquad (1.5)$$

Figure 1.5: Convective energy transport across a fluid element

1.4.2   Work associated with molecular motion

Recall from the first law of thermodynamics that the change in internal energy for a closed system can be represented by the following equation:

$$dU = dq + dW$$

Hence for flow systems, we are yet to account for the work done by molecular motion of fluids.

$$dW = F.dr$$

$$\frac{dW}{dt} = F.\frac{dr}{dt} = F.v$$

Since the forces appearing here are from molecular motion, we can use the molecular momentum flux to represent this force :

$$\frac{dW}{dt} = F.v = (\pi.dS).v$$

Recall that the molecular momentum flux is given by

$$\pi_{ij} = P\delta_{ij} + \tau_{ij}$$

Combined energy flux

Similar to how we defined the combined momentum flux tensor for momentum transport, we have a helpful combined energy flux *vector* (e) for energy transport.

$$\boxed{e = q + q^{(c)} + w} \tag{1.6}$$

q is the Fourier's law conduction term. Expanding the second and third terms, $q^{(c)} = (\frac{1}{2}\rho v^2 + \rho U)v$, $w = [\pi.v]$, giving us

$$e = q + (\frac{1}{2}\rho v^2 + \rho U)v + [\pi.v]$$

Since $\pi = P\delta + \tau$, we can use the definition $H = U + PV$ from thermodynamics to construct an alternate equation for e, as such :

$$e = q + (\frac{1}{2}\rho v^2 + \rho H)v + [\tau.v]$$

1.5   Demonstrating Mass Transport

1.5.1   Diffusive Transport

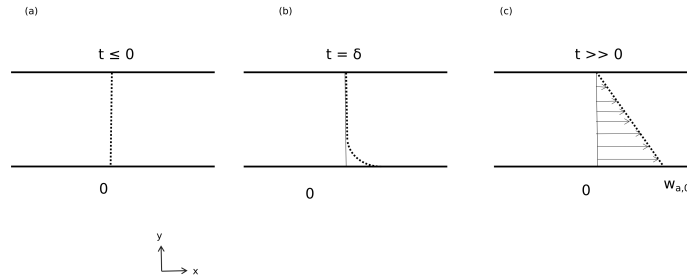Let us once again revisit our example of a fluid between two surfaces.

Figure 1.6: Helium diffusion across a silica slab

- Consider a silica slab. This silica slab can absorb helium, but not air. One end of this slab is at y = 0 and the other at y = Y as shown in figure 1.6. We are going to introduce some helium into this system eventually. We assume this slab is infinitely long and wide. The system is at equilibrium with air and there are no concentration gradients anywhere. Figure 1.6(a) shows how the concentration of helium is initially uniform at 0 every point between the two ends of silica.

- Now, let us see what happens when we attach a helium source of concentration w_{A0}. The concentration of helium in the silica near the lower end is now w_{A0}. This helium starts to disperse across the silica elements near the bottom of the slab.

- Figure 1.4(b) describes a snapshot of the system where some of the helium has started to go across to the silica near the lower end of the slab.

- Note that the top end is still exposed to the environment where we just have air and the helium concentration is taken to be 0. Over time, the helium atoms begin to diffuse steadily across the slab and the concentration along points the y direction go up eventually. Figure 1.4(c) showcases the steady-state concentration profile of the slab.

The steady state concentration profile to a good approximation is given by the following expression:

$$\frac{w_A}{A} = \rho \mathscr{D}_{AB} \frac{w_{A0}}{Y}$$

Here $\mathscr{D}$ is the diffusivity. If we extend this to each differential slice across the slab:

$$\boxed{j_{Ay} = -\rho \mathscr{D}_{AB} \frac{dw_A}{dy}} \tag{1.7}$$

Here, j_{Ay} is the mass flux.
This is called **Fick's Law of Diffusion**.
Some points to note :

- Here, $\mathscr{D}$ is the diffusivity. We write $\mathscr{D}_{AB}$ to indicate that we are describing the diffusivity of component A across a medium B.

- Unlike fluid velocity, which is a vector, concentration is a scalar quantity. Similarly, in momentum transport, τ was a tensor. Here j_A is a vector with components j_{Ax}, j_{Ay}, j_{Az}. These are mass fluxes in the directions perpendicular to the x, y and z axes. The multidimensional equivalent of Fourier's law is:

$$j_A = -\rho \mathscr{D}_{AB} \nabla w_A$$

1.5.2   Convective mass transport

As discussed before, transport can also occur with bulk fluid motions. Here let's look at mass transport for bulk fluid motions. Across a fluid element, let us think of the mass transport across a plane perpendicular to the x-axis (or parallel to the yz plane).

Let the convective mass transport be given by $j_A^{(c)}$. The mass per unit volume is the density ρ_A of component A. The x-component of convective mass flux is hence given by $j_{Ax}^{(c)} = \rho_A v_x dS$. In three dimensions this is $j_A^{(c)} = \rho_A \vec{v}$

1.5.3   Notation in mass transport

Since there are various ways of denoting concentration, velocity and flux in mass transport, it is important to have a glossary of all the notation.
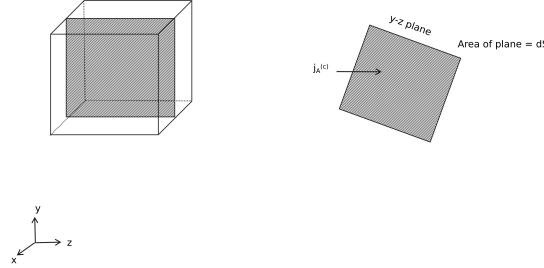
Figure 1.7: Convective mass transport across an element

Note that we will only be covering binary (or 2-component) systems here as the discussion of multi-component systems is very tricky and involves complicated expressions.

Some of the important equations and definitions you need to remember as follows:

- ρ_A is the mass of A per unit volume.

- $\rho = \rho_A + \rho_B$ is the mass density of the fluid mixture.

- $w_A = \frac{\rho_A}{\rho}$ is the mass fraction of A in the mixture.

- $w_A + w_B = 1$. Which means that $\nabla w_A = -\nabla w_B$.

- c_A is the number of moles of A per unit volume.

- $c = c_A + c_B$ represents the total molar concentration.

- $x_A = \frac{c_A}{c}$ is the mole fraction of A in the mixture.

- $x_A + x_B = 1$, which again means that $\nabla x_A = -\nabla x_B$.

- $\rho = cM$ where M is the molecular weight. This means that $w_A = \frac{x_A M_A}{M}$

- $\nabla w_A = \frac{M_A M_B \nabla x_A}{M^2} = \frac{w_A w_B \nabla x_A}{x_A x_B}$. This helps in converting representations of mass concentrations to molar concentrations and vice versa.

- v_A is the velocity of component A.

- The mass-average velocity v is given by $v = \frac{\rho_A v_A + \rho_B v_B}{\rho_A + \rho_B} = w_A v_A + w_B v_B$.

- The convective mass flux vector is given by $j_A^{(c)} = \rho_A v$.

- The molar-average velocity v^* is given by $v^* = x_A v_A + x_B v_B$.

- The convective molar flux vector is given by $J_A^{(c)} = c_A v^*$

- Fick's law in terms of mass-flux vector : $j_{Ay} = -\rho_A \mathscr{D}_{AB} \frac{dw_A}{dy}$.

- Fick's law in terms of molar-flux vector : $J_{Ay}^* = -c \mathscr{D}_{AB} \frac{dx_A}{dy}$.

Useful Dimensionless Groups in Mass Transport

- Prandtl Number $Pr = \frac{v}{\alpha} = \frac{C_p \mu}{k}$

- Schmidt Number $Sc = \frac{v}{\mathscr{D}_{AB}} = \frac{\mu}{\rho \mathscr{D}_{AB}}$

- Lewis Number $Le = \frac{\alpha}{\mathscr{D}_{AB}} = \frac{k}{\rho C_p \mathscr{D}_{AB}}$.

Combined flux vectors in mass transport

The combined mass-flux vector n_A is given by:

$$n_A = j_A^{(c)} + j_A = \rho_A v - \rho \mathscr{D}_{AB} \nabla w_A$$

The combined molar-flux vector N_A is given by:

$$N_A = J_A^{*(c)} + J_A^* = c_A v^* - c \mathscr{D}_{AB} \nabla x_A$$

For binary mixtures, the most useful expressions that can be used for the mass-flux and molar-flux vectors are:

$$\boxed{\begin{aligned} n_A &= w_A(n_A + n_B) - \rho \mathscr{D}_{AB} \nabla w_A \\ N_A &= x_A(N_A + N_B) - \rho \mathscr{D}_{AB} \nabla x_A \end{aligned}} \qquad \begin{aligned} (1.8) \\ (1.9) \end{aligned}$$

Chapter 2

Shell Balances

2.1 Shell Momentum Balances

Hello

2.2 Shell Energy Balances

2.3 Shell Mass Balances