UIT-RGPV (Autonomous) Bhopal
Department of Petrochemical Engineering

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Semester: VII

Subject code – PC 702 **Subject: Transport Phenomena**

Unit: -V
Lecture no.26

Mass transfer

1. Give significance of Brinkman number.

The **Brinkman Number** is a dimensionless group related to heat conduction from a wall to a flowing viscous fluid, commonly used in polymer processing. There are several definitions; one is

$$N_{Br} = \frac{\eta U^2}{\kappa(T_w - T_0)}$$

Where

N_{Br} (or Br)= the Brinkman Number

η = fluid viscosity (dynamic)

U = fluid velocity

κ = thermal conductivity of fluid

T_0 = bulk fluid temperature

T_w = wall temperature

Brinkman Number (Br)	$\frac{\mu v^2}{k(T-T_o)}$	Ratio of viscous dissipation to thermal conduction

In, for example, a screw extruder, the energy supplied to the polymer melt comes primarily from two sources (i) viscous heat generated by shear between parts of the flow moving at different velocities (ii) direct heat conduction from the wall of the extruder. The former is supplied by the motor turning the screw, the latter by heaters. The Brinkman Number is a measure of the ratio of the two.

2. **Write down the law of conservation of mass for a chemical species.**

"The mass in an isolated system can neither be created nor be destroyed but can be transformed from one form to another".

➢ **Formula of Law of Conservation of Mass**

Law of conservation of mass can be expressed in the differential form using the continuity equation in fluid mechanics and continuum mechanics as:

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

Where,

- ρ is the density
- t is the time
- v is the velocity
- ∇ is the divergence

Law of Conservation of Mass Examples

- **Combustion process:** Burning of wood is a conservation of mass as the burning of wood involves Oxygen, Carbon dioxide, water vapor and ashes.
- **Chemical reactions:** To get one molecule of H_2O (water) with the molecular weight of 10, Hydrogen with molecular weight 2 is added with Oxygen whose molecular weight is 8, thereby conserving the mass.

Conservative form of equations for reacting flows. Equations describing chemically reactive flows with N participating species in conservative formulation are stated as follows:

- Mass Conservation for Chemical Species:

$$\frac{\partial \rho Y_i}{\partial t} + \nabla \cdot (\rho Y_i \mathbf{v}) = -\nabla \cdot \mathbf{j}_i + w_i \quad (i = 1, 2, \cdots N) \tag{1}$$

- Mass Conservation for Mixture Gases:

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{v}) = 0 \tag{2}$$

- Conservation of Momentum:

$$\frac{\partial \rho \mathbf{v}}{\partial t} + \nabla \cdot (\rho \mathbf{v} \otimes \mathbf{v}) = -\nabla p + \nabla \cdot \boldsymbol{\tau} + \rho \sum_i^N Y_i \mathbf{f}_i \tag{3}$$

- Conservation of Energy

$$\rho \frac{\partial \rho e_t}{\partial t} + \nabla \cdot \{(\rho e_t + p)\mathbf{v}\} = -\nabla \cdot \mathbf{q} + \nabla \cdot (\boldsymbol{\tau} \cdot \mathbf{v}) + \rho \sum_i^N Y_i \mathbf{f}_i \cdot \mathbf{v} + \sum_i^N \mathbf{f}_i \cdot \mathbf{j}_i \tag{4}$$

$$e_t = h - \frac{p}{\rho} + \frac{1}{2}\mathbf{v} \cdot \mathbf{v} \tag{5}$$

- Thermodynamic Equation of State:

$$p = \rho R T M^{-1}, \quad M = \left(\sum_{i=1}^N Y_i / M_i \right)^{-1}, \tag{6}$$

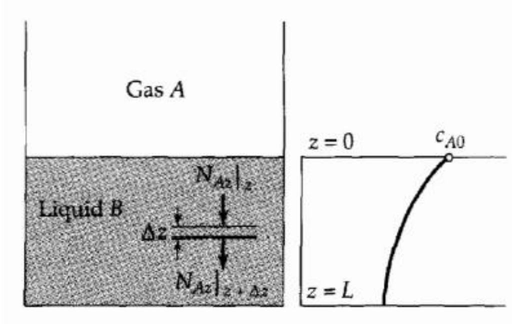
where ρ means the density, $\mathbf{v}$ denotes the velocity vector, p stands for the pressure, $\boldsymbol{\tau}$ represents the viscous tensor, $\mathbf{f}_i$ means the body force per unit mass of species i, Y_i represents the mass fraction of chemical species i, $\mathbf{j}_i$ denotes the diffusive flux vector of species i, w_i stands for the mass production rate of species i, e_t is the total energy, $\mathbf{q}$ denotes the heat flux vector, h represents the enthalpy, R is the universal gas constant, T denotes the temperature, M means the mean molecular mass, and M_i stands for the molecular mass of species i. The viscous stress tensor $\boldsymbol{\tau}$, the diffusive flux vector of species $\mathbf{j}_i$, and the heat flux vector $\mathbf{q}$ will be given in the section of "Constitutive equation".

3. Derive concentration profile for diffusion with homogeneous chemical reaction

Diffusion with a Homogeneous Chemical Reaction (e.g. Gas Dissolving in Liquid)

(1) Diffusion with a Homogeneous Chemical Reaction (e.g. Gas Dissolving in Liquid)

Problem: Consider a gas A diffusing into a liquid B. As it diffuses, the reaction $A + B \rightarrow AB$ occurs. You can ignore the small amount of AB that is present (this is the pseudobinary assumption).



1. Note that the reaction rate can be given as $k_1'''c_A$ if we assume pseudo-first order. This makes the shell mass balance
$$SN_{A,z}|_z - SN_{A,z}|_{z+\Delta z} - k_1'''c_A S\Delta z = 0$$
2. This can be rewritten as
$$\frac{dN_{A,z}}{dz} + k_1'''c_A = 0$$
3. If the concentration of A is small (i.e. dilute), then we can state that x_A goes to zero in
$$N_{A,z} = -c\mathscr{D}_{AB}\frac{dx_A}{dz} + x_A\left(N_{A,z} + N_{B,z}\right)$$
such that
$$N_{A,z} = -\mathscr{D}_{AB}\frac{dc_A}{dz}$$

4. Combining this with the equation in step 2 yields
$$\mathscr{D}_{AB}\frac{d^2c_A}{dz^2} - k_1'''c_A = 0$$

5. The boundary conditions are $c_A(0) = c_{A0}$ and $N_{A,z}(L) = \left.\frac{dc_A}{dz}\right|_L = 0$. The first boundary condition states that the concentration of A at the surface is fixed. The second boundary condition states that no A diffuses through the bottom of the container.

6. Multiply the equation in Step 4 by $\frac{L^2}{c_{A0}\mathscr{D}_{AB}}$ for later simplicity. This yields
$$\frac{L^2}{c_{A0}}\frac{d^2c_A}{dz^2} - \frac{k_1'''c_A L^2}{c_{A0}\mathscr{D}_{AB}} = 0$$

7. Let's define the dimensionless variable known as the Thiele modulus:

$$\phi \equiv \sqrt{k_1''' L^2 / \mathscr{D}_{AB}}$$

8. Let's also define the dimensionless length

$$\xi \equiv \frac{z}{L}$$

such that

$$dz = L d\xi$$

9. The concentration ratio ca be defined as

$$\Gamma \equiv \frac{c_A}{c_{A0}}$$

10. Using these variables,

$$\frac{d^2\Gamma}{d\xi^2} - \phi^2 \Gamma = 0$$

11. The general solution is given as

$$\Gamma = C_1 \cosh(\phi\xi) + C_2 \sinh(\phi\xi)$$

since

$$\cosh(p) \equiv \frac{e^p + e^{-p}}{2}$$

and

$$\sinh(p) \equiv \frac{e^p - e^{-p}}{2}$$

12. The boundary conditions are at $\xi = 0$, $c_A = c_{A0}$, so $\Gamma = 1$ and $\xi = 1$, $\frac{d\Gamma}{d\xi} = 0$. Applying boundary condition,

$$1 = C_1 \cosh(0) + C_2 \sinh(0) \rightarrow C_1 = 1$$

and

$$\frac{d\Gamma}{d\xi} = \phi \sinh(\phi\xi) + C_2 \phi \cosh(\phi\xi)$$

and invoking the second boundary condition yields

$$0 = \phi \sinh\phi + C_2 \phi \cosh\phi \rightarrow C_2 = -\tanh\phi$$

13. This yields

$$\Gamma = \cosh(\phi\xi) - \tanh(\phi)\sinh(\phi\xi)$$

which can be rearranged to[10]

$$\Gamma = \frac{\cosh(\phi)\cosh(\phi\xi) - \sinh(\phi)\sinh(\phi\xi)}{\cosh(\phi)} = \frac{\cosh[\phi(1-\xi)]}{\cosh\phi}$$

14. Reverting to the original notation yields,

$$\frac{c_A}{c_{A0}} = \frac{\cosh\left[\sqrt{k_1''' L^2/\mathscr{D}_{AB}}\left(1 - \frac{z}{L}\right)\right]}{\cosh\left(\sqrt{k_1''' L^2/\mathscr{D}_{AB}}\right)}$$

15. The average concentration in the liquid phase can be given by

$$\frac{\overline{c}_A}{c_{A0}} = \frac{\int_0^L \frac{c_A}{c_{A0}}\,dz}{\int_0^L\,dz} = \frac{\tanh\phi}{\phi}$$

16. The molar flux at the surface is

$$N_{A,z}\big|_{z=0} = -\,\mathscr{D}_{AB}\frac{dc_A}{dz}\bigg|_{z=0} = \left(\frac{c_{A0}\mathscr{D}_{AB}}{L}\right)\phi\tanh\left(\phi\right)$$

[10]Note that $\cosh\left(x \pm y\right) = \cosh x \cosh y \pm \sinh x \sinh y$ and $\sinh\left(x \pm y\right) = \sinh x \cosh y \pm \cosh x \sinh y$