

## Lecture 2

### Mass transfer and diffusion

*Mass transfer* is the net movement of a component in a mixture from one location to another where the component exists at a different concentration. In many separation operations, the transfer takes place between two phases across an interface. Thus, the absorption by a solvent liquid of a solute from a carrier gas involves mass transfer of the solute through the gas to the gas-liquid interface, across the interface, and into the liquid. Mass-transfer models describe this and other processes such as passage of a species through a gas to the outer surface of a porous, adsorbent particle and into the adsorbent pores, where the species is adsorbed on the porous surface. Mass transfer also governs selective permeation through a nonporous, polymeric material of a component of a gas mixture. Mass transfer, as used here, does not refer to the flow of a fluid through a pipe. However, mass transfer might be superimposed on that flow. Mass transfer is not the flow of solids on a conveyor belt.

Mass transfer occurs by two basic mechanisms: (1) molecular diffusion by random and spontaneous microscopic movement of individual molecules in a gas, liquid, or solid as a result of thermal motion; and (2) eddy (turbulent) diffusion by random, macroscopic fluid motion. Both molecular and/or eddy diffusion frequently involve the movement of different species in opposing directions. When a net flow occurs in one of these directions, the total rate of mass transfer of individual species is increased or decreased by this bulk flow or convection effect, which may be considered a third mechanism of mass transfer. Molecular diffusion is extremely slow, whereas eddy diffusion is orders of magnitude more rapid. Therefore, if industrial separation processes are to be conducted in equipment of reasonable size, fluids must be agitated and interfacial areas maximized. If mass transfer in solids is involved, using small particles to decrease the distance in the direction of diffusion will increase the rate.

When separations involve two or more phases, the extent of the separation is limited by phase equilibrium, because, with time, the phases in contact tend to equilibrate by mass transfer between phases. When mass transfer is rapid, equilibration is approached in seconds or minutes, and design of separation equipment may be based on phase equilibrium, not mass transfer. For separations involving barriers, such as membranes, differing species mass-transfer rates through the membrane govern equipment design.

In a binary mixture, molecular diffusion of component A with respect to B occurs because of different potentials or driving forces, which include differences (gradients) of concentration (ordinary diffusion), pressure (pressure diffusion), temperature (thermal diffusion), and external force fields (forced diffusion) that act unequally on the different chemical species present. Pressure diffusion requires a large pressure gradient, which is achieved for gas mixtures with a centrifuge. Thermal diffusion columns or cascades can be employed to separate liquid and gas mixtures by establishing a temperature gradient. More widely applied is forced

diffusion in an electrical field, to cause ions of different charges to move in different directions at different speeds.

In this lecture, only molecular diffusion caused by concentration gradients is considered, because this is the most common type of molecular diffusion in separation processes. Furthermore, emphasis is on binary systems, for which molecular-diffusion theory is relatively simple and applications are relatively straightforward. Diffusion in multicomponent systems is much more complex than diffusion in binary systems, and is a more appropriate topic for advanced study using a text such as Taylor and Krishna [I].

Molecular diffusion occurs in solids and in fluids that are stagnant or in laminar or turbulent motion. Eddy diffusion occurs in fluids in turbulent motion. When both molecular diffusion and eddy diffusion occur, they take place in parallel and are additive. Furthermore, they take place because of the same concentration difference (gradient). When mass transfer occurs under turbulent-flow conditions, but across an interface or to a solid surface, conditions may be laminar or nearly stagnant near the interface or solid surface. Thus, even though eddy diffusion may be the dominant mechanism in the bulk of the fluid, the overall rate of mass transfer may be controlled by molecular diffusion because the eddy-diffusion mechanism is damped or even eliminated as the interface or solid surface is approached.

Mass transfer of one or more species results in a total net rate of bulk flow or flux in one direction relative to a fixed plane or stationary coordinate system. When a net flux occurs, it carries all species present. Thus, the molar flux of an individual species is the sum of all three mechanisms. If  $N_i$  is the molar flux of species  $i$  with mole fraction  $x_i$ , and  $N$  is the total molar flux, with both fluxes in moles per unit time per unit area in a direction perpendicular to a stationary plane across which mass transfer occurs, then

$$N_i = x_i N + \text{molecular diffusion flux of } i + \text{eddy diffusion flux of } i$$

where  $x_i N$  is the bulk-flow flux. Each term is positive or negative depending on the direction of the flux relative to the direction selected as positive. When the molecular and eddy-diffusion fluxes are in one direction and  $N$  is in the opposite direction, even though a concentration difference or gradient of  $i$  exists, the net mass-transfer flux,  $N_i$  of  $i$  can be zero.

The subject of mass transfer and diffusion is divided into seven areas: (1) steady-state diffusion in stagnant media, (2) estimation of diffusion coefficients, (3) unsteady-state diffusion in stagnant media, (4) mass transfer in laminar flow, (5) mass transfer in turbulent flow, (6) mass transfer at fluid-fluid interfaces, and (7) mass transfer across fluid-fluid interfaces.