CHAPTER III

THEORY

3.1 Theories of Ordinary Diffusion in Liquids.

3.1.1The Hydrodynamical Theory

The Nernst-Einstein equation states that the diffusivity of a single particle or solute molecule of A through a stationary medium B is.

$$D_{AB} \quad = \quad (\kappa T \ \mu_A) / F_A \ \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots(3.1)$$

which μ_A/F_A is the “mobility” of the particle of A.

$$F_A \quad = 6 \ \pi\mu_A \ \mu_B \ R_A . \text{ (Stokes' Law)}$$

and Stokes - Einstein equation gives.

$$D_{AB} \ \mu_A / \kappa T \quad = \quad (1/6)\pi R_A \qquad \ldots\ldots\ldots\ldots\ldots\ldots\ldots(3.2)$$

which has been shown to be fairly good for describing the diffusion of large spherical particles or large spherical molecules in dilute solution and also for the coefficient of self-diffusion.

Diffusion through a nonisothermal spherical film.

$$(D_{AB}/D_{AB1}) \quad = \quad (T/T_1)^{3/2} \ldots\ldots\ldots\ldots\ldots\ldots\ldots(3.3)$$

3.1.2 Eyring-Rate Theory

On the assumption of a cubic lattice configuration, this theory gives the following relation between the self-diffusion coefficient and the coefficient of viscosity.

$$D_{AB}\,\mu_B / \kappa T = (N / V_A)^{1/3} \qquad \text{.......................(3.4)}$$

Wilke has developed a correlation for diffusion coefficients on the basis of the Stoke-Einstein equation. His results may be summarized by the following approximate analytical relation , which gives the diffusion coefficient in $cm^2\ sec^{-1}$ for small concentrations of *A* in *B*.

$$D_{AB} = 4.4x10^{-8}\,((\psi M_B)^{1/2}\,T) / \mu\, V^{0.6} \qquad \text{.......................(3.5)}$$

This equation is good only for dilute solutions of nondissociating solute, for such solution it is usually good within ± 10 percent.

3.2 Fick Rate Equation

3.2.1 Fick's First Law of Diffusion [23]

Whithin binary isothermal system of species *A*, *B* Bird, Stewart and Lightfoot [20] proposed the definition of an unidirectional diffusion.

$$N_A = -cD_{AB}\,(dX_A/dZ) + X_A(N_A + N_B) \qquad \text{.........................(3.6)}$$

The diffusion flux N_A, relative to stationary coordinates, is the resultant of two vectors quantities.

The vector $X_A(N_A + N_B)$ is the molar flux of A resulting from the bulk motion of fluid.

The vector $-cD_{AB}(dX/dZ)$ is the molar flux of A resulting from the diffusion superimposed on the bulk flow.

The equation (3.1) is the general definition of diffusivity. If the substance *A* is slightly soluble, $X_A(N_A + N_B)$ term is neglected.

$$N_A = -cD_{AB}\,(dX_A/dZ) \qquad \text{...(3.7)}$$

which is Fick's first law.

3.2.2 Fick's second Law of Diffusion [22]

Transient process, in which the concentration at agiven point varies with time, are referred to as unsteady-state processes or time dependent processes. The time-dependent differential equations are simple to derive from the general differential equation for mass transfer.

The equation of continuity for component A,

$$\nabla \cdot N_A + (\partial C_A / \partial t) - R_A = 0 \qquad \text{......................(3.8)}$$

Many solutions are for one-directional mass transfer as defined by Fick's second " law " of diffusion,

$$(\partial C_A / \partial t) = D_{AB}(\partial^2 C_A / \partial Z^2) \qquad \text{.....................(3.9)}$$

This equation is well known Fick's second Law of diffusion.

3.3 "Standard Turbine" Design

The designer of an agitated vessel has an unusually large number of choices to make as to type and location of the impeller, the proportions of the vessel, the number and proportions of the baffles, and so forth. Each of these decisions affects the circulation rate of the liquid, the velocity patterns, and the power consumed. As a starting point for design in ordinary agitation problems, a turbine agitator of the type shown in Fig. is commonly used. Typical proportions are

$d = D/2$ $\qquad$ $b = D/5$

$l = D/4$ $\qquad$ $n_P = 6$

$H = D$ $\qquad$ $C = H/6\text{-}H/3$

$B_w = 0.1D$ $\qquad$ $n_B = 4$

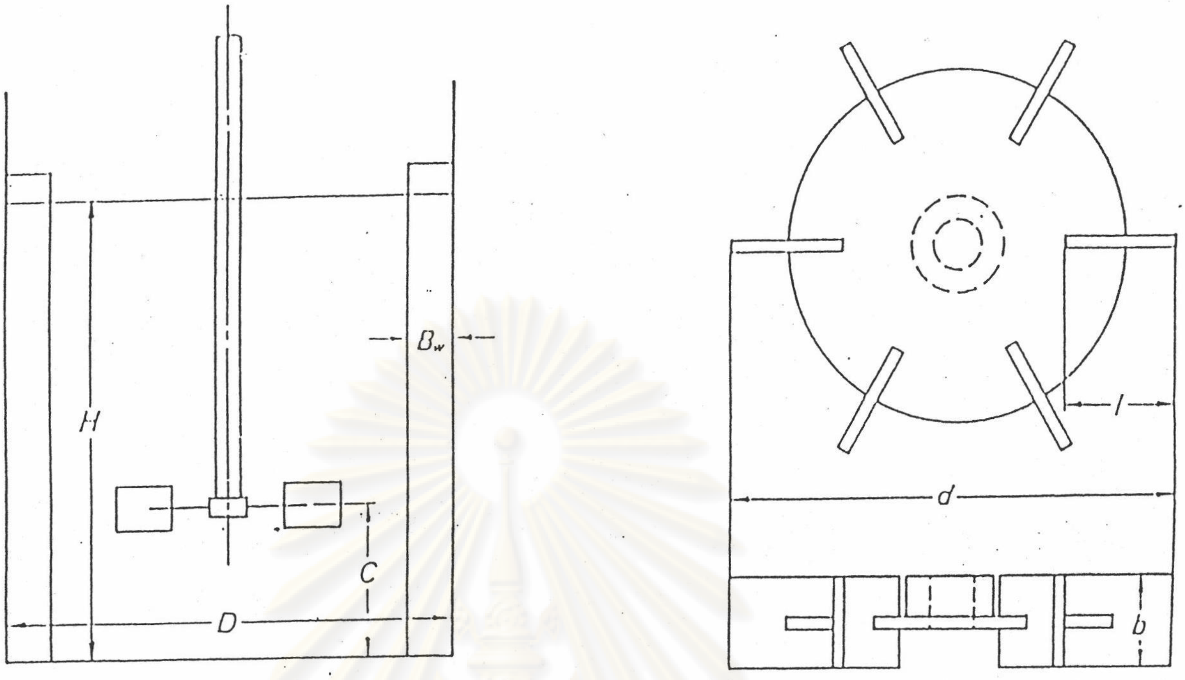

Figure 3.1: Standard 6-Blade Turbine Impeller & Agitated Tank [21]

The number of baffles is usually 4; the number of impeller blades ranges from 4 to 16 but is generally 6 or 8. Special situations may, of course, dictate different proportions from those listed above; it may be advantageous, for example, to place the agitator higher or lower in the tank, or a much deeper tank may be needed to achieve the desired process result. The listed "standard" proportions, nonetheless, are widely accepted and are the basis of many published correlations of agitator performance.

3.4 Solid-Liquid Mass Tranfer[12]

A study of solid-liquid mass transfer considers the effect of mixing on the surface area of the solids (which is often a minimal effect) and the effect of mixing on the fluid film around the solid particles.

Three major correlation methods have been tried by various investigators. One method, using dimensional analysis, usually takes the form:

$$kT/D_v = rRe_T\ Sc \qquad \text{.........................(3.14)}$$

or

$$kT/D_v = rRe_a\ Sc \qquad \text{.........................(3.15)}$$

where Re_T = Reynolds number referred to tank

Sc = Schmidt number

Re_a = Reynolds number referred to agitator

Several investigators have tried using this equation in their correlations, but the constant r and exponents *p* and *q* vary with impeller type and system geometry. Therefore, other geometric ratios and groups are needed, as well as the functional relationships between correlating parameters.

A second method involves the particle Sherwood number kd_p/D_v as a function of particle Reynolds number and Schmidt number.

The third correlation method is based on the slip velocity and terminal velocity of the particle. In a reactor in which the solid particles are fully suspended, Harriott [16] showed that the relative particle liquid velocity is related to, and is always greater than the free-fall terminal velocity of the solid particles in static liquid.

3.5 Flow Pattern in Agitated Vessel

The type of flow in an agitated vessel depends on the type of impeller, the characteristics of the fluid, and the size and proportions of the tank, baffles, and impeller. The velocity of the fluid at any point in the tank has three components, and the overall flow pattern in the tank depends on the variations in these three velocity components from point to point. The first velocity component is radial and acts in a direction perpendicular to the shaft of the impeller. The second component is longitudinal and acts in a direction parallel with the shaft. The third component is tangential, or rotational, and acts in a direction tangent to a circular path around the shaft. In the usual case of a vertical shaft, the radial and tangential components are in a horizontal plane, and the longitudinal component is vertical. The radial and longitudinal components are useful and provide the flow necesssary for the mixing action. When the shaft is vertical and centrally located in the tank, the tangential component is generally disadvantageous. The tangential flow follows a circular path around the shaft, creates a vortex at the surface of the liquid, as shown in Fig.3.2, and tends to perpetuate, by a laminar-flow circulation, stratification at the various levels without accomplishing longitudinal flow between levels.If solid particles are present, circulatory currents tend to throw the particles to the outside by centrifugal force, from where they move downward and to the center of the tank at the bottom. Instead of mixing, its reverse, concentration, occurs. Since, in circulatory flow, the liquid flows with the direction of motion of the impeller blades, the relative velocity between the blades and the liquid is reduced and the power that can be absorbed by the liquid is limited. In an unbaffled vessel circulatory flow is induced by all types of impellers, whether axial flow or radial flow. In fact, if the swirling is strong, the flow pattern in the tank is virtually the same regardless of the design of the impeller. At high impeller speeds the vortex may be so deep that it reaches the impeller, and gas from above the liquid is drawn down into the charge. Generally this is undesirable.

3.6 Impeller Types [22]

3.6.1 Impellers

Impellers are divided into two classes : those which generate currents parallel with the axis of the impeller shaft and those which generate currents in a tangential or radial direction. The first are called axial-flow impellers, the second radial-flow impellers.

The three main types of impellers are propellers, paddles, and turbines. Each type includes many variations and subtypes, which will not considered here. Other special impellers are also useful in certain situations, but the three main types solve perhaps 95 percent of all liquid-agitation problems.

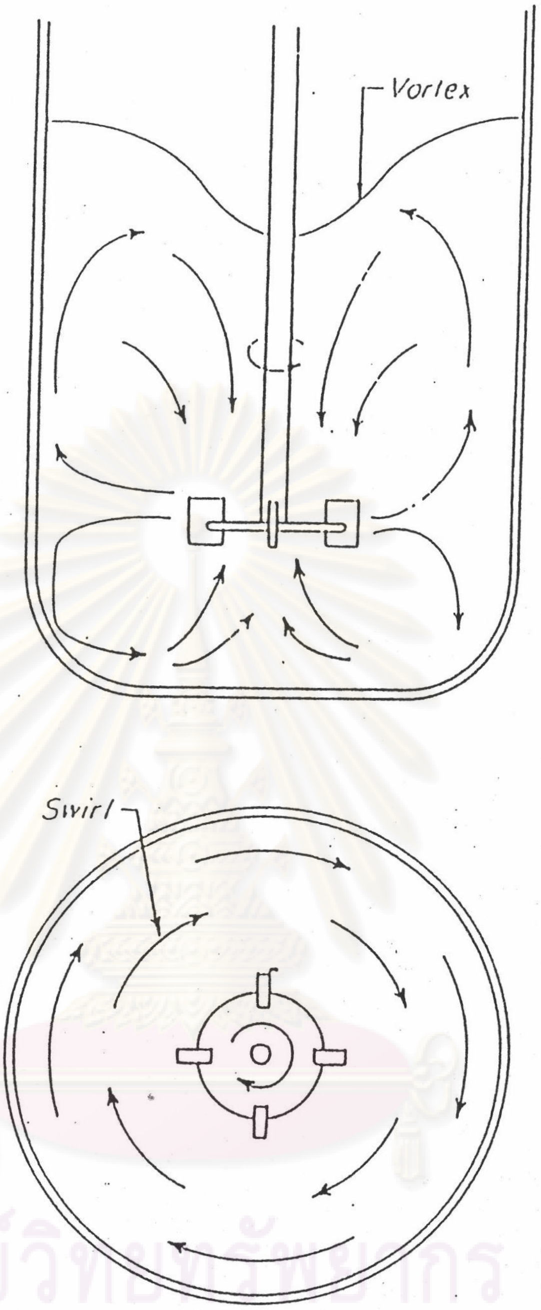

Figure 3.2 : Vortex formation and circulation pattern in an agitated tank[22]

3.6.2 Propellers

A propeller is an axial-flow, high-speed impeller for liquids of low viscosity. Small propellers turn at full motor speed, either 1,150 or 1,750 rpm. larger ones turn at 400 to 800 rpm.The flow currents leaving the impeller continue through the liquid in a given direction until deflected by the floor or wall of the vessel. The highly turbulent swirling column of liquid leaving the impeller entrains stagnant liquid as it moves along, probably considerably more than an equivalent column from a stationary nozzle would. The propeller blades vigorously cut or shear the liquid. Because of the persistence of the flow currents, propeller agitators are effective in very large vessels.

A revolving propeller traces out a helix in the fluid, and if there were no slip between liquid and propeller, one full revolution would move the liquid longitudinally a fixed distance depending on the angle of inclination of the propeller blades.The ratio of this distance to the propeller diameter is known as the pitch of the propeller. A propeller with a pitch of 1.0 is said to have square pitch.

A typical propeller is illustrated in Fig. 3.3 Standard three bladed marine propellers with square pitch are most common; four-bladed, toothed, and other designs are employed for special purposes.

Propellers rarely exceed 18 in. in diameter regardless of the size of the vessel. In a deep tank two or more propellers may be mounted on the same shaft, usually directing the liquid in the same direction. Sometimes two propellers work in opposite directions, or in "push-pull," to create a zone of especially high turbulence between them.

3.6.3 Paddle

For the simpler problems an effective agitator consists of a flat paddle turning on a vertical shaft. Two-bladed and four-bladed paddles are common. Sometimes the blades are pitched; more often they are vertical. Paddles turn at slow to moderate speeds in the center of a vesssel; they push the liquid radially and tangentially with almost no vertical motion at the impeller unless the blades are pitched.The currents they generate travel outward to the vessel wall and then either upward or downward. In deep tanks several paddles are mounted one above the other on the same shaft. In some designs the blades conform to the shape of a dished or hemispherical vessel so that they scrap the surface or pass over it with close clearance. A paddle of this kind is known as an anchor agitator. Anchors are useful for preventing deposits on a heat-transfer surface, in a jacketed process vessel, but they are poor mixers. They nearly always operate in conjunction with a higher-speed paddle or other agitator, usually turning in the opposite direction.

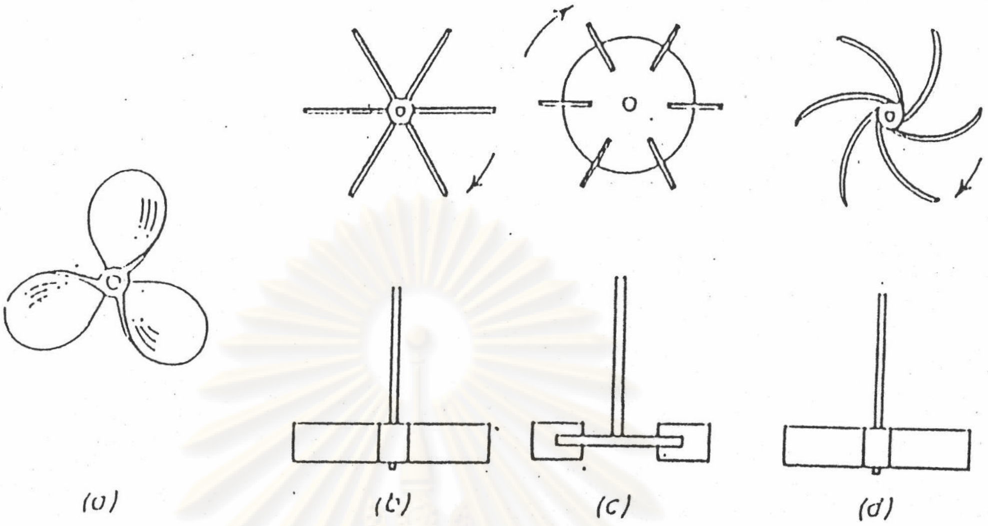

Figure 3.3 : Mixing impellers [22]

(a) three-bladed marine propeller (b) open straight-blade turbine
(c) bladed disk turbine (d) vertical curved-blade turbine.

Industrial paddle agitators turn at speeds between 20 and 150 rpm. The total length of a paddle impeller is typically 50 to 80 percent of the inside diameter of the vesssel. The width of the blade is one-sixth to one-tenth its length. At very slow speeds a paddle gives mild agitation in an unbaffled vessel; at higher speeds baffles become necessary. Otherwise the liquid is swirled around the vessel at high speed but with little mixing.

3.6.4 Turbines

Some of the many designs of turbine are shown in Fig.3.3 b,c and d. Most of them resemble multibladed paddle agitators with short blades, turning at high speeds on a shaft mounted centrally in the vessel.The blades may be straight or curved, pitched or vertical. The impeller may be open, semienclosed or shrouded. The diameter of the impeller is smaller than the paddles, ranging from 30 to 50 percent of the diameter of the vessel.

Turbines are effective over a very wide range of viscosities. In low-viscosity liquids turbines generate strong currents which persist throughout the vesssel, seeking out and destroying stagnant pockets. Near the impeller is a zone of rapid currents, high turbulence, and intense shear.The principal currents are radial and tangential.The tangential components induce vortexing and swirling, which must be stopped by baffles or by a diffuser ring if the impeller is to be most effective.

3.7 Suspension of Solid Particles in Agitated Liquids[21]

The state of suspension of solid particles in liquids is not usually homogeneous, since nonuniformity is observed due to the unevenness of liquid velocities. Therefore we should consider two criteria;

1) the critical agitator speed, N_f, at which all the solid particles are suspended, and
2) the uniformity of local concentration of the slurry.

The most common application in mixing technology. The state of complete suspension of solid particles in liquid refers to the instant at which all solids are in circulation and none is resting on the vessel bottom.Suspension of solids in a liquid medium will be obtained when the uising velocity of the liquid phase equal or exceeds the settling velocity of the particles. Fluid velocity and direction are function of impeller selection and of vessel configuration. Particle setting velocity is a function of gravitation force, fluid drag, properties of solid (i.e.density, size, shape), solid concentration and several hindering factors such as viscosity difference.