

Diffusion

Diffusion gas, liquid, solid phase or sometimes interphase mass in systems with multiple phase transfer mechanism. For example, Let's think water of several crystals of a coloring agent such as copper sulfate that it is placed in a long bottle filled with. One color in the bottle first we see that it begins to spread and that this color is concentrated at the bottom of the bottle. After a day we observe that the color penetrates a few centimeters upwards. If a sufficiently long period of time (several years) is expected, the solution may be observed to have a homogeneous color.

The process is responsible for the movement of the colored material. Diffusion is responsible for the movement of the colored material. Diffusion is a result of the random movement of molecules in all directions, and these random movements provide a complete crosstalk. Diffusion is a slow process. While the diffusion rate in gases is 10 cm / min, it is about 0.05 cm / min in liquids and 0.00001 cm / minute in solids. In general, the diffusion rate varies with temperature less than other events.

The fact that the diffusion rate is slow the main reason for diffusion to gain importance. Mostly in the system according to a certain order with other processes to form a diffusion mechanism takes place.

The slowest step in this sequence determines the speed of the process. For example, the distillation efficiency and Penicillin producing rates of absorption of industrial substances using porous catalysts the rate of growth of microorganisms, the rate of corrosion of the steel, and the rate of spread of nutrients from the nutrients always control the diffusion rate. The diffusion rate in gases and liquids can be increased by mixing. For example, copper sulfate in a vial for a long period of time may be completely mixed in a few minutes if it is mixed. This speed increase is not only due to diffusion but a combination of diffusion and mixing. Diffusion is still a phenomenon of molecules that occur in small molecules distances. Mixing molecules are not a process. However, it can carry the fluid to a very large distance as an anesthetic process.

The definition of diffusion involves a mathematical model based on a basic hypothesis or "law". There are two common approaches to such a law. A more basic diffusion coefficient is the Fick's diffusion law. This law is commonly used to determine diffusion. The second approach involves the use of a mass transfer coefficient, which can be considered as a kind of reversible speed coefficient, which is not a generic name. Which of these two models is chosen depends on the system conditions.

Determination of Diffusion Coefficient in Gases

In the binary gas mixture, the diffusion coefficient can be calculated from gas kinetic theory in the dilution zone, i.e. at or near atmospheric pressure. In this theory, it is assumed that the gases are composed of hard spherical particles and their collisions with the other particles are a fully elastic work that shows that the momentum is preserved. It is assumed that there is no thrust and pulling forces between the molecules.

A more accurate and elaborate approach involves pushing and pulling forces between molecules of A and B, take into account that they may have molecules of different sizes. Chapman and Enskog solved the Boltzmann equation, which uses a distribution function on the average free path. The solution of this equation requires the use of a correlation between the propulsion and tensile forces of a given pair of molecules. Lennard Jones function is an acceptable approach for non-polar molecule pairs.

Expression of diffusion constant for molecule pair A and B:

$$D_{AB} = \frac{1,8583 * 10^{-7} * T^{3/2}}{P * \sigma_{AB} * \Omega_{D,AB}} \left(\frac{1}{M_A} + \frac{1}{M_B} \right)^{1/2}, m^2 / s$$

Here;

D_{AB} : Diffusion constant m^2/s

M_A, M_B : Molecular weigh of gases A and B, kg/kgmol

σ_{AB} : Average collision radius

$\Omega_{D,AB}$: A collision integral depend on Lennord-Jones potantial.

Diffusion in liquids

The diffusion coefficient in the liquids has a semi-empirical structure since no complete theory can be established for the diffusion in liquids. One of the first theories of Stokesinst Einstein equation is a small molecule solvent (B) is produced for the diffusion of a large molecule solute (A). Soluble substance this equality, in which the Stoke law is used to determine the drift over the molecules It is arranged according to the fact that the molecules have similar and cubic cell structure.

$$D_{AB} = \frac{9,96 * 10^{-6} * T}{\mu V_A^{1/3}}$$

Here;

D_{AB} : Diffusion constant m^2/s

T : Temperature, K

μ : Viscosity, Pa.s or kg/m.s

V_A : Molar volúme of solute at the normal boiling point, m^3/kg

This equation is dehydrated, spherical, large molecule, having a molecular weight of about 1000 or greater It gives very accurate results for solutes or substances with molar volume of 0.5 $m^3 / kgmol$.

For smaller molar volumes, this equation does not give the correct results. Various other theoretical approaches have been used, but accurate results have been obtained. The Wilkela Chang correlation can be used for more general purposes.

$$D_{AB} = 1,173 * 10^{-16} * (\phi_B * M_B)^{1/2} * \frac{T}{\mu_B * V_A^{0,6}}$$

Here;

ϕ : association parameter for the solvent. For water 2,6 methanol 2,9, ethanol 1,5 and for similar of benzene, ether, heptane 1,0

Diffusion in Porous Solids

Porous solids in mass transfer operations to provide a large surface area per unit volume are widely used. For example, in hydro refining processes in petroleum refineries, as a catalyst in the removal of

CO, NO, and unburned hydrocarbons in automobile exhaust gases or porous with different diameters from 1 mm to 15 mm on fixed bed filled columns use of solids as catalysts or adsorbents from numerous engineering applications just a few.

Diffusion in porous solids; molecular diffusion, Knudsen diffusion and surface diffusion mechanisms. Solid pores as mentioned by Fick's Law on Molecular Diffusion It is the diffusion mechanism that dominates when the gas is relatively large and relatively dense.

When the pores are small or the gas density is low, the molecules are interconnected with the pore walls they collide more often than they do. Therefore, diffusion of molecules along the pore, free molecules can be indicated by the equations obtained for flow. In this diffusion Knudsen diffusion It is called. Both collisions at middle pressures and pore sizes (they play an important role in the diffusion of molecules. Same time certain molecules are adsorbed on the walls of the pores; It is molecular moving and wall they diffuse in the direction of decreasing surface concentration. Surface diffusion, molecular diffusion and Knudsen diffusion rates are very small and very small diffusion mechanism.

It is a generally accepted approach that the transport for mass transfer within the catalysts can be given by a linear correlation in the following, with acceptable accuracy in many engineering applications.

$$J_A = -c * D_{A,eff} \nabla X_A$$

Here, the sub-index eff efficient means, diffusivity is considered the presence of solid material. shows. Molecular diffusion and Knudsen diffusion are approximately equally important and are simply considered collectable resistances.

$$\frac{1}{D_{A,eff}} = \frac{1}{D_{AB,eff}} + \frac{1}{D_{KA,eff}}$$

Surface diffusion may be neglected as the pores of the catalyst tablets are relatively large. Effective diffusivity can be obtained as follows.

$$D_{AB,eff} = \frac{\varepsilon}{\tau} D_{AB}$$

In the equation, D_{AB} , the double diffusion coefficient in the Fick's Law, the ε porosity or the volume fraction of the solid (to take into account the decrease in the cross-sectional area due to the presence of the solid) and the bending factor is τ Factor. Knudsen active diffusivity is;

$$D_{KA,eff} = \frac{\varepsilon}{\tau} D_{KA}$$

Knudsen diffusion coefficient from D_{KA} , for A matter, free molecular flow theory

$$D_{KA} = \frac{2}{3} * \Gamma * v_A$$

can be calculated from the equation. Here. Is the effective pore radius and the average molecular velocity in the V_A . For average molecular speed;

$$V_A = \left(\frac{8 * R * T}{M_A} \right)^{1/2}$$

Via placing the value of the gas constant R;

$$D_{KA} = 9 * \Gamma * \left(\frac{T}{M_A} \right)^{1/2}, m^2 / s$$

At atmospheric pressure, if the pore radius is greater than 2µm, molecular diffusion is dominant and Knudsen diffusion is dominant if the pore radius is less than 0.2 µm.

Perparations for the experiment

1. In what cases is the diffusion coefficient, in which cases the mass transfer coefficient is used?
2. What is the Graham diffusion law?
3. Compare the diffusion rates in solids, liquids and gases.
4. What are the effects of pressure and temperature on the diffusion rate in solid, liquid and gas gases?
5. Fick's diffusion law with Newton's viscosity and Fourier's thermal conductivity laws compare to what extent is the similarity between these three correlations valid?
6. Stokes y Einstein equation gives the correlation between the stack properties?
7. Compare the relationship between DAB and ies for gases and liquids.
8. A non-zero VXA in a two-component system means that the molar flux NA is not zero will it come? Please explain.
9. Compare Ni with Ji to ni and jiregard as physical significance.
10. The equivalent inverse diffusion of the molar flux relation for Aand B is (NA =-NB). Find two special forms for diffusion of A into the stagnant B.