Lecture №5. Classification of solids

Aim: Analyze the classification of materials in the solid phase. Give an equation to determine the diffusion coefficient. Discussion of criterion equations.

Lecture summary: Based on the analysis of the structural and kinetic properties of materials constituting the solid phase, a unified classification of the solid phase - distributed substance systems is proposed (table 1).

In the external phase, substance transfer can be carried out by molecular, convective, and turbulent diffusion. The general laws of substance transfer in the liquid and gas phases were considered earlier. If the external environment is stationary, then Fick's law of molecular diffusion (1) is used to describe diffusion in a stationary medium, which occurs as a result of random movement of molecules.

Values of the diffusion coefficients of gases under normal conditions are given in reference books. Recalculation of other conditions can be performed by the equation:

$$D = D_o \left(\frac{T}{T_o}\right)^{1,5} \left(\frac{P_o}{P}\right), \qquad (19)$$

where D_o – the diffusion coefficient under normal conditions (T_o = 272 K, P_o = 101,325 kPa). Diffusion coefficients in liquids are calculated using various empirical equations.

The transfer of the substance to be distributed from one point of space to another in a moving medium is carried out not only by molecular diffusion, but also by the transport of a substance by a moving medium (convective diffusion). Therefore, the distribution of the concentration of this component in a stationary moving medium, with unsteady mass transfer process, is described by the differential equation of convective diffusion (6).

In the turbulent flow of the external phase, the transfer of substance in the transverse (with respect to the flow) direction is carried out not only by molecular diffusion, but also by the migration of chaotic vortices generated by internal friction between the fluid layers and obeying static laws. Turbulent diffusion is described by equation (1a). The convective diffusion equation, which also takes into account molecular and turbulent diffusion, will be:

$$\frac{\partial C_c^{'}}{\partial r} = div[(D + \varepsilon_d) grad C_c^{'}] - \vec{\omega} grad C_c^{'}, \qquad (20)$$

where $C_c^{'}$ – the mass concentration of the substance to be distributed in the external phase, kg/m^3.

As mentioned earlier, the mass transfer coefficient β_c is determined from the corresponding criterial dependences obtained by the methods of the similarity theory. At the boundary with the solid phase, the mass transfer intensity can be expressed both by the molecular diffusion equation (1) and the convective diffusion equation (6).

If D and $\vec{\omega}$ are not constant, the solution of equation (6) is unknown. Then the methods of the theory of similarity are used. The methods of the similarity theory give the following criteria: a) Reynolds: $Re = \frac{\omega l}{\nu}$; b) Prandtl mass-exchange: $Pr_m = \frac{\nu}{D}$; c) the Nusselt mass-exchange: $Nu_m = \frac{\beta_c l}{D}$.

Table 1

Classification of solid phase materials

Number, class name and its classification	Group number and its sign	Examples of materials
1. Non-porous materials (internal mass transfer is determined by the laws of migration of the molecules of the distributed substance between the molecules of a solid body).	1) Non-porous materials, the transfer of substances in which obeys the law of molecular diffusion of Fick.	Polyamides-6, -66, -610, -12, polyethylene terephthalate, polypropylene, polycarbonate, dried from water.
	2) Non-porous materials, the transfer of the dispersed substance in which is characterized by anomalous diffusion.	Polystyrene or cellulose acetate containing methylene chloride or chloroform, PVA and gelatin containing water.
2. Capillary-porous materials (transport of the substance to be distributed occurs through the pore system).	1) Capillary-porous materials with a fixed porous structure.	Silica gel, active alumina, zeolites, active carbons, two-water gypsum, calcined ceramics, metal ceramics.
	2) Capillary-porous materials with a pore structure that changes during the process of mass transfer.	Porous material containing solid phase, removed by extraction; wet layer of bulk material.
3. Colloidal capillary-porous materials (porous materials with permeable pore walls).	1) Colloidal capillary-porous materials in which the transfer of the substance to be distributed through the colloidal component of the skeleton of the body obeys Fick’s law.	Ceramic masses.
	2) Colloidal capillary-porous materials in which mass transfer through the colloidal parts of the body framework is characterized by anomalous diffusion.	Celluloid containing ethyl alcohol.

The general criterial equation has the form: $Nu_m = f(Re, Pr_m, Fo_m)$.

For stationary conditions, the Fourier criterion Fo_m falls out, and the criterion equation takes the following basic form: $Nu_m = f(Re, Pr_m)$.

The criterion Pr_m for gases will vary in the range 0,5-3,0 (for humid air 0,55-0,6), for liquids Pr_m = 1-10^4. For the coefficient of turbulent diffusion ε_d, the following approximate relation holds: ε_d = Re.

In the case that it is necessary to take into account the influence of additional factors – natural convection, liquid evaporation conditions, gravity or surface tension –– appropriate criteria are also used: a) Archimedes: $Ar = \frac{gl^3}{\nu^2} \cdot \frac{\Delta\rho}{\rho_s}$; b) Grashof: $Gr = \frac{gl^3}{\nu^3}(T_m - T_{s.s})$; c) Gukhman: $Gu = \frac{T_m - T_{w.t}}{T_m}$, where l – the defining linear dimension, m; ρ_m – medium density, kg/m^3; ν – kinematic viscosity, m^2/s; T_m, $T_{s,s}$, $T_{w,t}$ – respectively, the temperature of the medium, the surface of the solid and the wet thermometer.

For technical purposes, the values of the mass emission (output) coefficients averaged over the surface of a solid body find the greatest application. Calculation of these values for specific cases (flat surface, single bodies, fixed or fluidized bed) is carried out using appropriate criterion dependencies.

Questions to control:

1. Bring and analyze the classification of materials in the solid phase.
2. Write an equation to determine the diffusion coefficient.
3. Give equations for calculating the diffusion similarity criterion.

Literature:

1. Ishanhodjaeva M.M. Physical chemistry. Part 1. Diffusion in systems with a solid phase. - SPb.: SPbGTURP, 2012. - 35 p.

2. Tsvetkov S.K. Mass transfer processes in systems involving the solid phase. - SPb.: SPbU, 2017. - 50 p.

3. Kasatkin A.G. Basic processes and devices of chemical technology. – M: Alliance, 2006. – 752 p.

4. Romankov P.G., Frolov V.F., Flisyuk O.M. Calculation methods of processes and devices in chemical technology (examples and tasks). – St.-Petersburg: Himizdat, 2011. – 544 p.