Lecture 8 «The modified equation of a mass transfer. Mass-exchange between phases. Convective diffusion. Criteria equation of a convective mass-exchange»

Aim: Formulate and write the modified equation of a mass transfer. Describe the mass-exchange between phases. Describe the convective diffusion. Formulate the criteria of diffusion similarity.

Lecture summary: Modified equation of mass transfer. In many cases of computational practice, the basic mass transfer equation is used in a modified form. Since the phase contact surface is not determined by a simple geometric calculation. In this case, the main technical characteristic of the apparatus can be the volume, height or number of stages of phase contact.

To derive a modified mass transfer equation, when the main technical characteristic of the apparatus is taken to be its height, the phase contact surface in the entire volume of the apparatus can be represented by the expression:

$$F = fH\sigma, \, m^2, \tag{1}$$

where f – the sectional area of the apparatus, m^2, H – the height of the apparatus, m^2, σ – the specific surface area of the phase contact per unit volume of the apparatus, m^2/m^3.

Substituting the found values of the phase contact surface (1) into the basic mass transfer equation, we obtain

$$M = K_y fH\sigma \frac{y_{in}-y_f}{\int_{y_f}^{y_{in}} \frac{dy}{y-y^*}} \tag{2}$$

Replacing

$$M = G(y_{in} - y_f), \tag{3}$$

will have

$$G(y_{in} - y_f) = K_y fH\sigma \frac{y_{in}-y_f}{\int_{y_f}^{y_{in}} \frac{dy}{y-y^*}}, \tag{4}$$

Whence

$$H = \frac{G}{K_y f\sigma} \int_{y_f}^{y_{in}} \frac{dy}{y-y^*} \tag{5}$$

If the driving force is expressed through the concentration of the distributed substance in the liquid phase, the modified mass transfer equation (5) will have the form:

$$H = \frac{L}{K_x f\sigma} \int_{x_{in}}^{x_f} \frac{dx}{x^*-x} \tag{6}$$

where L and G – the flows of liquid and gas entering to the treatment.

The multipliers in equations (5) and (6) $\frac{G}{K_y f \sigma}$, $\frac{L}{K_x f \sigma}$ represent the height of the apparatus section corresponding to one transport unit and is called the transfer unit height ($TUH = h$).

The integral is the change in the working concentration per unit of driving force in a given section and is called the number of transfer units – n. The number of transfer units is determined by the method of graphical integration. One transfer unit $n = 1$ corresponds to the section of the apparatus in which the change in operating concentrations is equal to the average driving force in a given section.

Equations (5) and (6) after the introduction of a certain height of transfer units and the number of units of transfer are written down [2, 3].

$$H = hn \tag{7}$$

Mass exchange between phases

The transfer of substance between phases is carried out simultaneously by molecular and convective diffusion. In the mass of the phase, due to intensive mixing, the concentration of the distributed substance in each section of the system is almost identical, and therefore the transport of substance is carried out predominantly by convective diffusion, i.e. moving particles of the carrier and the substance being distributed.

In the boundary layer, substance is transported by both by molecular and convective diffusion. At the phase interface, the role of molecular diffusion increases. If mass transfer occurs between a solid phase and a liquid or gas, then the substance is transported inside the solid phase by mass conductivity. The law of mass conductivity is analogous to the law of molecular diffusion.

The transfer of substance by molecular diffusion is determined by Fick's first law, according to which the amount of substance diffused through the layer is proportional to the concentration, time, and surface gradient of the layer perpendicular to the direction of the diffusion flow,

$$dM = -D \frac{\partial c}{\partial x} dF d\tau, \tag{8}$$

where M – the amount of diffused substance, kg (kgf); $\frac{\partial c}{\partial x}$ – concentration gradient in the diffusion direction $(kg/m^3)/m^2$; F – the area of the layer through which the substance diffuses, m^2; τ – the time, s (h); D – the diffusion coefficient.

The proportionality coefficient D in the Fick's law expression is called the molecular diffusion coefficient, or simply the diffusion coefficient. The minus sign in front of the right-hand side of Fick's first law indicates that molecular diffusion always proceeds in the direction of decreasing the concentration of the distributed component.

The dimension of the diffusion coefficient is determined from the Fick's equation (8):

$$[D] = \left[\frac{dM \partial x}{dF \partial c \partial \tau}\right] = \left[\frac{kg \cdot m}{m^2 \cdot kg/m^3 \cdot s}\right] = \left[\frac{m^2}{s}\right] \tag{9}$$

or in the MKGSS system

$$[D] = \left[\frac{dM\partial x}{dF\partial c\partial \tau}\right] = \left[\frac{kgf \cdot m}{m^2 \cdot kgf/m^3 \cdot h}\right] = \left[\frac{m^2}{h}\right] \qquad (10)$$

The diffusion coefficient shows how much substance diffuses per unit time through a unit surface with a concentration gradient of unity.

Returning to the analogy with the processes of heat distribution, it can be noted that the diffusion coefficient D is an analog of the coefficient of temperature conductivity a.

The molecular diffusion coefficient is a physical constant that characterizes the ability of a given substance to penetrate due to diffusion into a stationary environment. The value D thus does not depend on the hydrodynamic conditions in which the process proceeds.

The value of the diffusion coefficient D is a function of the properties of the substance being distributed, of the properties of the environment through which it diffuses, temperatures and pressures. Usually, the values D increase with increasing temperature and a decrease in pressure (for gases). In each specific case, the value of the diffusion coefficient is determined from experimental data or from theoretical and semiempirical equations, taking into account the temperature and pressure at which the diffusion process takes place [2, 3].

Convective diffusion

In convective diffusion, substance is transported by moving particles of the carrier and the substance being distributed.

With convective diffusion, the amount of the transferred substance from the phase giving up the substance to the phase interface is proportional to the surface of the phase contact, time, the particular driving force, i.e. the difference in the concentration of the distributed substance in the phase and at the interface:

$$dM = \beta dF d\tau \Delta c, \qquad (11)$$

where F – the phase contact surface, m²; τ – the time, s; Δc – the private driving force of the process; β – the mass emission coefficient.

The mass emission coefficient shows how much mass of substance passes from the interface of phases to the core of the phase (or in the opposite direction) through unit of surface per unit time with a driving force equal to unity.

The mass emission coefficient is not a physical constant, but a kinetic characteristic that depends on the physical properties of the phase (density, viscosity, etc.) and the hydrodynamic conditions in it (laminar or turbulent flow regime), which in turn are related to the physical properties of the phase, factors determined by the design and dimensions of the mass exchange apparatus.

In terms of meaning, the mass emission coefficient is an analog of the heat emission coefficient in heat transfer processes, and the basic mass emission equation is identical in structure to the basic heat emission equation.

The mass emission coefficient can be expressed in various units, depending on the choice of units for the mass of the substance to be distributed and the driving force.

The dimension of the mass emission coefficient is determined from the equation of convective diffusion (11):

$$[\beta] = \left[\frac{dM}{dFd\tau\Delta c}\right] = \left[\frac{kg}{m^2 \cdot s \cdot (u.driv.force)}\right] \qquad (12)$$

If the working and equilibrium concentrations of the substance to be distributed are expressed in terms of relative weight compositions (kg/kg), then the mass emission coefficient dimension will be:

$$[\beta] = \left[\frac{dM}{dFd\tau\Delta c}\right] = \left[\frac{kg}{m^2 \cdot s \cdot kg/kg}\right] = \left[\frac{kg}{m^2 \cdot s}\right] \qquad (13)$$

When expressing the driving force (for the gas or vapor phase) through the difference in partial pressures $\Delta p = p - p^*$, N/m²:

$$[\beta] = \left[\frac{dM}{dFd\tau\Delta c}\right] = \left[\frac{kg}{m^2 \cdot s \cdot N/m^2}\right] = \left[\frac{kg \cdot s^2 \cdot m^2}{m^2 \cdot s \cdot kg \cdot m}\right] = \left[\frac{s}{m}\right] \qquad (14)$$

If the driving force of the process is expressed in terms of the difference in volume concentrations (kg/m³), then the dimension of the mass emission coefficient will be [2, 3]:

$$[\beta] = \left[\frac{dM}{dFd\tau\Delta c}\right] = \left[\frac{kg}{m^2 \cdot s \cdot kg/m^3}\right] = \left[\frac{m}{s}\right] \qquad (15)$$

Criteria of diffusion similarity

Criteria for diffusion (mass-exchange) similarity are obtained from the basic equation of convective-diffusion mass transfer of a component in a single-phase flow:

$$\frac{\partial C}{\partial \tau} + w_x \frac{\partial C}{\partial x} + w_y \frac{\partial C}{\partial y} + w_z \frac{\partial C}{\partial z} = D \left(\frac{\partial^2 C}{\partial x^2} + \frac{\partial^2 C}{\partial y^2} + \frac{\partial^2 C}{\partial z^2}\right) \qquad (16)$$

or in compact vector form

$$\frac{\partial C}{\partial \tau} + (\vec{w}, grad\, C) = D\nabla^2 C, \qquad (17)$$

where the convective terms are represented by the scalar product of the velocity vector $\vec{w}$ and the gradient of concentration *grad C*, and the diffusion ones – by the Laplace operator $\nabla^2 C$.

To derive the similarity criteria from equation (16), this equation is written in a simplified, one-dimensional form with the notation of the spatial coordinate replaced by *l*. Then, instead of (16), we write

$$\frac{\partial C}{\partial \tau} + w \frac{\partial C}{\partial l} = D \frac{\partial^2 C}{\partial l^2}, \qquad (18)$$

where the principal physical content of the equation (16) and its individual terms is completely preserved.

The right-hand side of equation (18), corresponding to the transport intensity of the target component due to molecular diffusion, is divided into the first term of the left side, which reflects the overall rate of change of the component concentration at an arbitrary point of the carrier stream:

$$D \frac{\partial^2 C}{\partial l^2} / \frac{\partial C}{\partial \tau} \sim D \frac{(C_i - C_0)}{l^2} / \frac{(C_i - C_0)}{\tau} = \frac{D\tau}{l^2}, \tag{19}$$

where C_i – the concentration of the component at the interface; C_0 – the concentration of the component in the bulk of the carrier stream.

In this case we obtain a dimensionless complex of quantities

$$\frac{D\tau}{l^2} = Fo_D, \tag{20}$$

which is called the diffusion Fourier's criterion.

The diffusion Fourier's criterion is a measure of the ratio of the rate of change in concentration caused by molecular diffusion to the total overall rate of change in concentration at any point of the moving environment. By analogy with non-stationary processes of conductive-convective heat transfer, the diffusion Fourier's criterion is often called the dimensionless time of the nonstationary diffusion-convective mass transfer of the component.

The division of the convective term of (18) into a diffusion term and the analogous replacement of the derivatives with respect to the coordinate by the ratio of finite differences gives another independent criterion for diffusion similarity, known as the Peclet's diffusion criterion:

$$w \frac{\partial C}{\partial l} / D \frac{\partial^2 C}{\partial l^2} \sim w \frac{(C_i - C_0)}{l} / \left(D \frac{(C_i - C_0)}{l^2} \right) = \frac{wl}{D} = Pe_D \tag{21}$$

The Peclet's diffusion criterion is a measure of the ratio of the intensity of transfer of a component by convection and the transfer by molecular diffusion.

By multiplying and dividing by the kinematic viscosity of the environment, the Peclet's diffusion criterion can be represented in terms of the Reynolds criterion and a new criterion – the Prandtl's diffusion criterion (Schmidt's criterion):

$$Pe_D = \frac{wl}{D} \frac{v}{v} = \frac{wl}{v} \frac{v}{D} = RePr_D \tag{22}$$

The Prandtl's diffusion criterion is a measure of the ratio of the viscosity and diffusion properties of the environment carrier:

$$Pr_D = \frac{v}{D} = \frac{\mu}{\rho D} \tag{23}$$

Prandtl's diffusion criterion includes only quantities reflecting the physical properties of the flow. Thus, this criterion formally expresses the constancy of the ratio of the physical properties of the liquid (gas) at similar points of similar flows. However, its physical

meaning is deeper, as the viscosity is determined, with all other conditions being equal, the velocity profile in the flow, and the concentration distribution depends ultimately on the value D.

Another criterion of diffusion similarity, important for practical calculations, is obtained from an analysis of the mass exchange conditions at the phase interface. Since the amount of substance moving from the phase to the phase boundary is determined by the convective diffusion equation (11), at the interface of the phases this same amount of substance moves to another phase due to molecular diffusion and is determined by the molecular diffusion equation. The mathematical formulation of the boundary conditions can be written in the form:

$$\beta(C_{bd} - C_0) = D(\partial C / \partial n), \tag{24}$$

where n – the direction along the normal to the wall.

The left-hand term is divided by the right, then the unknown value of the derivative $\partial C / \partial n$ is replaced by the proportional ratio of the concentration difference $(C_{bd} - C_0)$ to the characteristic geometrical dimension of the system l:

$$\beta(C_{bd} - C_0) = \left[D \left(\frac{\partial C}{\partial n} \right) \right] \sim \frac{\beta(C_{bd}-C_0)[D(C_{bd}-C_0)]}{l} = \beta l / D \tag{25}$$

Diffusion criterion Nusselt (Sherwood):

$$Nu_D = \frac{\beta l}{D} \tag{26}$$

is a measure of the ratio of the mass emission rate from the surface to the intensity of diffusion transfer. In its structure, the Nusselt's diffusion criterion is completely analogous to the Nusselt's heat criterion, which characterizes the heat exchange at the boundary.

Experimental data on the determination of the mass emission coefficients β are processed and represented as a dependence of the Nusselt's diffusion criterion on the defining Reynolds criteria, the Prandtl's diffusion criterion, and for nonstationary processes – also on the diffusion Fourier's criterion:

$$Nu_D = f(Re, Pr_D, Fo_D) \tag{27}$$

For stationary processes, a Fourier's criterion consisting of the current time τ is excluded from the set of defining criteria:

$$Nu_D = f(Re, Pr_D) \tag{28}$$

If there are zones or points with different densities $\Delta\rho$ in the volume of the environment, then the Archimedes's criterion is introduced into the set of defining criteria, and for geometrically inconvenient systems geometric simplices G_1, G_2, ... are added.

Thus, the experimental data on the intensity of mass exchange are presented in the form of a dependence of the Nusselt's number on the determining criteria and simplices of geometrical similarity:

$$Nu_D = f(Re, Pr_D, Ar, G_1, G_2, \cdots) \qquad (29)$$

The dependence (29) can be represented in power form:

$$Nu_D = ARe^m Pr_D^n G_1^k, \cdots \qquad (30)$$

The numerical values A, m, n, k in the criterion equation (30) are found experimentally, and the mass emission coefficient is determined from the Nusselt's diffusion criterion [1, 2].

$$\beta = \frac{Nu_D D}{l} \qquad (31)$$

Questions to control:
1. Derive the modified mass transfer equation if the driving force is expressed through the concentration of the substance distributed in the liquid phase.
2. Formulate Fick's first law.
3. What does the coefficient of molecular diffusion depend on? What is its physical meaning? What is its dimension?
4. What are the main differences in the transport of substance by convection and mass emission?
5. Expand the physical meaning of the mass-emission coefficient.
6. Give all possible dimensions of the mass-emission coefficient.
7. What is the physical content of the equation (16) for the convective-diffusion transfer of a component in a single-phase flow?
8. Describe the similarity of mass-exchange processes.
9. Write down the criterial mass emission equation for unsteady and steady mass transfer processes.
10. Expand the physical meaning of the similarity criteria for mass-exchange processes.

Literature
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