MODELING OF MASS TRANSFER IN CONTINUOUS AND DISPERSED PHASES DURING DROPLET MOTION IN EXTRACTORS

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Based on the Landau-Levich model of a diffusion boundary layer, the mass transfer in continuous and dispersed phases of two immiscible liquids is described mathematically. Basic parameters of the model are calculated in terms of the hydraulic resistance in droplet motion.

A mathematical description of the mass and heat transfer processes in two-phase media necessitates taking into account complex hydrodynamic conditions, in which these processes proceed and which are the factors governing the transfer rate. In most cases, the local velocities, the tangential stresses, and the interfacial area of two-phase flows in the working zone of a device are not known, and, therefore, the problem is often solved empirically. This leads to an increase in time and cost of the design of industrial units.

The current study has attempted to obtain, within the framework of a unified approach [1-3], a mathematical description of the mass transfer during free droplet motion in extractors.

The mass and heat transfer in dispersed flows may be represented by three stages, viz., transfer in the period of droplet formation, free motion of the elements of the dispersed medium in the working zone of the device, and coalescence. In some cases, the material transfer in the period of droplet formation may amount to 50-90% of the total transferred mass [4-6], and the mathematical modeling of an "inlet effect" is then of great importance. However, dimensions of the industrial unit and the velocity of the phase motion are in many cases such that the major portion of the material under the extraction conditions is extracted over the time of free motion of the droplets.

It is well known that a turbulent uniphase flow along a smooth solid surface commences at Reynolds numbers larger than 10^4 . The droplet motion occurs at smaller values of Re_d, which, at first sight, allows one to regard the boundary layer on the interface as laminar. However, the hydrodynamic regularities of the motion of two-phase media in many cases differ appreciably from the hydrodynamics of uniphase flows.

Disturbing factors (turbulence sources) in the two-phase media may be subdivided into two classes. The first is internal sources, viz., a mobile interface, a wave formation at the interface, a Marangoni effect, and a number of other factors [7-9]. To the second class we may assign turbulence caused by a mechanical agitation, and by a pulsatory or a vibrational motion of the medium in the working zone of the extractor. Therefore, it may be assumed that, in real conditions, the droplet boundary layer is nearly always disturbed by turbulent pulsations, increasing the rate of the mass and heat transfer.

The droplet motion in industrial extractors is effected, as a rule, when $\text{Re}_d \gg 1$, which corresponds to Peclet numbers $\text{Pe} > 10^3$. This allows consideration of the transfer processes based on the diffusion layer model.

If the process is limited by the dispersed phase, the diffusion boundary layer forms inside the droplet. In the course of time the mean concentration inside the droplet will begin to change noticeably, but in many cases the mass transfer coefficients can be calculated in the framework of a stationary boundary layer model [10] with accuracy sufficient for practical purposes.

Statement of the Problem. Let us write a mass flux in the boundary layer of dispersed and continuous phases with allowance for molecular and turbulent transfer

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$$j = (D + D_t) \frac{dC}{dy}.$$
(1)

Based on expression (1), resistance to the mass transfer in the boundary layer of thickness δ is presented in the form

$$\frac{1}{\beta} = \frac{(C_{\infty} - C_{\rm in})}{i} = \int_{0}^{0} \frac{dy}{(D + D_{\rm t})}.$$
(2)

For the coefficient $D_t(y)$, various power functions of the distance to the interface are employed [1-3, 11-13]. The range of application of such functions is generally bounded by the thickness of the viscous sublayer in the turbulent boundary layer. However, the structure of the boundary layer on the droplet interface differs from the structure of the classical turbulent boundary layer, and the range of application of these functions is not known. In this case, we proceed as follows: we use familiar power functions $D_t(y)$ in a viscous sublayer of the turbulent boundary layer, whereas their operation region (the thickness δ in expression (2)) is found from the fulfillment of the condition of momentum balance in the boundary layer on the droplet interface [14].

Modeling of the Mass Transfer in a Continuous Phase (external problem). If the rate of the diffusion process is limited by the rate of mass exchange in the continuous phase, then the magnitude of the mass flux is dependent on the hydrodynamics of the external flow and on the physical properties of the continuous medium.

The mass transfer in the continuous phase during stationary motion of the droplet with a Peclet number $Pe = V_{\infty}d_d/D > 10^3$ is usually examined in the framework of the diffusion boundary layer model. The resistance to the mass transfer in the boundary layer of the continuous phase has the form (2), where a decay law $D_t(y)$ is used as the power function [1-3, 11, 12]:

$$D_{t_2} = U_{*2} \delta_2 (y/\delta_2)^n.$$
(3)

For systems with a mobile interface and with a ratio of viscosities of dispersed and continuous phases $\mu^* = \mu_d/\mu_c < 1$ there is a relation $\beta \sim D^{1/2}$, and then the exponent in expression (3) is also equal to n = 2 according to the established relationship [2, 3] $\beta \sim D^{(n-1)/n}$. In this case, Eqs. (2) and (3) yield [2]

$$\beta_2 = \frac{U_{*2}}{\operatorname{arctg} \sqrt{R_{\delta 2} \operatorname{Sc}_2} \sqrt{R_{\delta 2} \operatorname{Sc}}}.$$
(4)

If the viscosity ratio of the droplet and the continuous medium is much greater than unity, the droplet motion is similar to the motion of a solid particle ($U_{in} = 0$). Here, the dependence of the mass transfer coefficient on the molecular diffusion coefficient is close in form to $\beta \sim D^{2/3}$, and in expression (3), n = 3. This also holds for systems with surfactants.

At n = 3, the expression for β appears as [3]

$$\beta_{2} = \frac{6\sqrt{3}U_{*2}L^{2}}{\sqrt{3}\ln\frac{(L+1)^{2}}{L(L+1)+1} + 6\operatorname{arctg}\frac{2-L}{\sqrt{3}L} + \pi},$$
(5)

where $L = (R_{\delta 2}Sc)^{1/3}$.

The parameter $R_{\delta 2}$ in the droplet boundary layer will be found from the known character of the momentum transfer [14]. The resistance to the momentum transfer is presented analogously to Eq. (2)

$$\frac{1}{\gamma_2} = \frac{\rho_2 \Delta \overline{U}_{\infty_2}}{\tau} = \int_0^{\delta_2} \frac{dy}{(v + v_t)_2},$$
(6)

where $\Delta \bar{U}_{\infty 2} = \bar{U}_{\infty 2} - \bar{U}_{in}$ is the mean motive force of the momentum transfer, m/sec.

Assuming the turbulent Schmidt number to differ insignificantly from unity, the coefficient $\nu_{t2}(y)$ is taken in the form (3), viz., $\nu_{t2} \approx D_{t2}$.

Expression (6) is integrated for n = 2 to give the value of the parameter $R_{\delta 2}$ in the boundary layer of the continuous phase

$$R_{\delta 2} = \left\{ \frac{\Delta U_{\infty 2}}{U_{*2} \operatorname{arctg} \sqrt{R_{\delta 2}}} \right\}^2.$$
⁽⁷⁾

For n = 3, the integration of expression (6) yields

$$R_{\delta 2} = \left\{ \frac{6 \sqrt{3} \Delta \bar{U}_{\infty 2}}{U_{\ast 2} \left(\sqrt{3} \ln \frac{(B+1)^2}{B(B+1)+1} + 6 \arctan \frac{2-B}{B\sqrt{3}} + \pi \right)} \right\}^{3/2},$$
(8)

where $B = (1/R_{\delta 2})^{1/3}$.

Modeling of Mass Transfer in a Dispersed Phase (internal problem). When the mass transfer process is limited by the dispersed phase, the boundary layer originates inside the droplet.

The condition of turbulent diffusion decay in the boundary layer of the dispersed phase on a mobile interface is taken in the form of the relation [11, 12]

$$D_{t1} = U_{*1} y_1^2 / \lambda_1, \tag{9}$$

where λ_1 is the minimal curvature radius of the surface deformation, defined as $\lambda_1 = 2\sigma/(\rho_1 U_{*1}^2)$.

From expressions (2) and (9) we derive the equation to determine the mass transfer coefficient

$$\frac{1}{\beta_1} = \frac{2\sigma}{\rho_1 U_{*1}^3 \delta_1} \frac{1}{\sqrt{a_1}} \operatorname{arctg} \psi_1 \sqrt{\frac{1}{a_1}} \Big|_0^1, \qquad (10)$$

where $\psi_1 = y_1/\delta_1$ and $a_1 = 2D_1\sigma/U_{*1}^3\delta_1^2\rho_1$. Hence

$$\beta_{1} = \sqrt{\frac{\overline{U_{\ast 1}\rho_{1}D_{1}}}{2\sigma}} \frac{U_{\ast 1}}{\operatorname{arctg}} \sqrt{\frac{U_{\ast 1}}{\operatorname{Sc}_{1}} \frac{U_{\ast 1}R_{\delta 1}^{2}\nu_{1}\rho_{1}}{2\sigma}}}.$$
(11)

To define the parameter $R_{\delta 1}$, we present the resistance to the momentum transfer in the boundary layer of the dispersed phase similarly to Eq. (2)

$$\frac{1}{\gamma_1} = \frac{\rho_1(\overline{U}_{\infty 1} - \overline{U}_{p})}{\tau} = \int_0^0 \frac{dy}{(\mathbf{v} + \mathbf{v}_t)_1}.$$
(12)

Assuming that the turbulent Schmidt number differs little from unity, we present the turbulent viscosity coefficient $v_{t1}(y)$ in the form (9), viz., $v_{t1} \approx D_{t1}$. As a result of integrating Eq. (12) we obtain

$$R_{\delta 1} = \sqrt{\frac{2\sigma}{\nu_1 \rho_1 U_{*1}}} \operatorname{tg}\left(\Delta \overline{U}_{*1} \sqrt{\frac{\nu_1 \rho_1}{2\sigma U_{*1}}}\right). \tag{13}$$

The motive force of the momentum transfer $\Delta \bar{U}_{\infty} = \bar{U}_{\infty 1} - \bar{U}_{in}$ for the boundary layer inside the droplet is determined by the difference in the liquid velocities on the interface \bar{U}_{in} and in the core $\bar{U}_{\infty 1}$. From the condition of symmetry of the velocity field we have $\bar{U}_{\infty 1} = 0$ for the droplet core, and then $\Delta \bar{U}_{\infty} = \bar{U}_{in}$.

Determination of Basic Parameters of the Model. Among the basic parameters of the derived model are the dynamic velocity U_* and the velocity on the droplet interface \overline{U}_{in} .

In the case of nonseparated flow past the droplet ($\text{Re}_d \leq 100$ [15]), from the condition of balance of the forces, when a pressure drop is equilibrated with a friction force on the interface, we have

$$U_{*1} = V_{\infty d} \bigvee \frac{\rho_2 \xi_d}{\rho_1 8}, \quad U_{*1} = V_{\infty d} \bigvee \frac{\xi_d}{8}.$$
(14)



Fig. 1. The dimensionless complex $Sh/Sc^{\frac{1}{2}}$ as a function of Re_d in extraction of different systems: 1, 2) calculation from Eq. (4); 3, 4) experimental data [17]; 1, 3) the water (continuous phase)-aniline-xylene system; 2, 4) the water (continuous phase)-benzoic acid-benzene system.

Fig. 2. The relation for the mass transfer coefficient in a dispersed phase in extraction of the amyl alcohol-phenol-water system, the dispersed phase is water: 1) calculation from Eq. (11); 2) experimental data [17]; $\mu^* = 1.73$; $D_1 = 0.84 \times 10^{-9} \text{ m}^2/\text{sec. }\beta$, m/sec.

If $\text{Re}_d > 100-200$, a separation of the boundary layer is observed in the trailing part, and Eqs. (14) give a significant error. The dynamic velocity for $\text{Re}_d > 200$ is expressed in terms of the energy dissipation in the dispersed phase using the familiar relation

$$\varepsilon = \tau \, \frac{dU}{dy} = U_{*1}^2 \rho_1 \, \frac{dU}{dy},\tag{15}$$

where the derivative is found from the equation $\tau = \rho_1(\nu + \nu_t) dU/dy$. Hence

$$s = \frac{U_{*1}^{4}\rho_{1}}{(\nu + \nu_{t})_{1}} = \frac{\tau^{2}}{\rho_{1}(\nu + \nu_{t})_{1}}.$$
(16)

Adopting the well-known assumptions of Prandtl that the momentum flux τ across the boundary layer is a constant value and utilizing the function $\nu_{t1}(y)$ (9), we find the mean energy dissipation

$$\overline{\mathbf{s}} = \frac{U_{\ast 1}^4 \rho_1}{R_{\delta 1} \mathbf{v}_1} \sqrt{\frac{2\sigma}{U_{\ast 1} \mathbf{v}_1 \rho_1}} \operatorname{arctg} \sqrt{\frac{R_{\delta 1}^2 \mathbf{v}_1 \rho_1 U_{\ast 1}}{2\sigma}}.$$
(17)

Hence we obtain mean values of the dynamic velocity in the dispersed

$$U_{*1} = \left[\frac{\overline{sv_1}R_{\delta 1}}{\rho_1} \sqrt{\frac{U_{*1}v_1\rho_1}{2\sigma}} \frac{1}{\arctan\left(\frac{R_{\delta 1}^2v_1\rho_1U_{*1}}{2\sigma}\right)} \right]^{1/4}$$
(18)

and continuous phases $U_{*2} = U_{*1}(\rho_1/\rho_2)^{\frac{1}{2}}$.

The mean energy dissipation over the droplet volume is presented in terms of the pressure drop or the resistance coefficient

$$\overline{\varepsilon} = \frac{\Delta P \pi R_d^2 V_{\infty d}}{4/3\pi R_d^3} = \frac{3}{8} \xi_d \frac{\rho_1 V_{\infty d}^3}{R_d}.$$
(19)

Therefore, the dynamic velocity in the boundary layer of the dispersed or continuous phases may be computed from the solution of Eqs. (13) and (16) with the parameters \bar{U}_{in} and $\bar{\epsilon}$ (19). The value of \bar{U}_{in} at small Reynolds numbers may be predicted using the Adamar-Rybchinskii function [10].



Fig. 3. The dimensionless complex Sh/Sc^{1/2} as a function of Re_d in extraction of the water-acetic acid-benzene system; the dispersed phase is benzene: 1) calculation from the mathematical model; 2) calculation from empirical expressions [18]; 3) experimental data [17]; $\mu^* = 0.65$; D₁ = 1.77 × 10⁻⁹ m/sec.

The mean velocity on the droplet interface for $Re_d >> 1$ is found from the balance equations of the forces written for the droplet and the solid particle at identical conditions of motion in the continuous medium.

It is well known [15, 16] that, owing to the interface mobility, the droplet floats up at a velocity higher than that of a solid particle of the same size, with other conditions being equal. This results from the fact that the condition of liquid attachment ($U_{in} = 0$) is fulfilled at the surface of the solid body. At the liquid-liquid interface a relative motion of the phases occurs, if μ^* is insignificantly larger than unity. Therefore, in the motion of the solid particle, velocity gradients at its surface are greater than in the boundary layer during the droplet flotation under similar conditions, and the resistance coefficient of the solid particle is larger than that of the droplet. In the region of a steady motion of the droplet the resistance coefficient decreases with rising Re_d number, remaining all the time lower than the resistance coefficient of the solid sphere.

It may be assumed that the velocity of the droplet is higher than that of the solid particle by the value of the mean velocity of the liquid at the interface $U_{in} \approx V_{\infty d} - V_{\infty s}$. In this case, the balance equations of forces, written for the droplet and the sphere, yield the following expression:

$$U_{\rm in} = V_{\infty d} \left(1 - \sqrt{\frac{\xi_d}{\xi_s}} \right) \quad \text{for} \quad \xi_d < \xi_s.$$
⁽²⁰⁾

As Re_d increases due to the droplet deformation, the resistance coefficient ξ_d starts to rise, attaining the value of the resistance coefficient for the solid sphere ξ_s , and afterwards exceeds its value by severalfold [15]. The resistance minimum is at Re_d ≥ 200 . In this case we assume that the mean velocity of the liquid at the droplet interface varies insignificantly with increasing Re_d number, and its value may be taken as at Re_d ≈ 200 , if the Reynolds number is larger than this value.

Empirical expressions [15-17] are recommended for the resistance coefficients of the droplet and the solid sphere at different Re_d.

Main Results and Deductions. The mathematical model developed is verified by comparing the mass transfer coefficients (4) and (11) with experimental data of various authors [17, 18].

Figure 1 gives the complex $Sh/Sc^{\frac{1}{2}}$ as a function of Re_d in extraction of different systems when the mass transfer process is limited by a continuous phase.

Equation (11) is checked in calculating the mass transfer coefficients in the dispersed phase over the Reynolds number range Re_d = 60-700 at $\mu^* = 0.65$ -1.75 and Sc = 570-848.

Figures 2 and 3 present correlations of the calculated results and the experimental data.

The agreement with experimental data in most cases lies within $\pm (15-20)\%$.

The derived equations allow calculation of the mass transfer coefficients in extractors with input of the external energy to the contacting phases. The mean value of the dissipated energy is determined in this case by the ratio of the power expended on agitation, as well as on vibrational and pulsatory motion of the phases, to the working volume of the two-phase medium.

The mathematical model given may be recommended for computing the kinetic characteristics of two-phase turbulent flows using only results of the hydraulic investigation of contact devices.

NOTATION

 C_{∞} , C_{in} , substance concentration in the phase core and at the interface; d_d , droplet diameter, m; D, D_t, coefficients of molecular and turbulent diffusion, m²/sec; j, mass flux; ΔP , pressure drop, Pa; R_{δ} , dimensionless thickness of the boundary layer; R_d , droplet radius, m; U_{*}, dynamic velocity of friction, m/sec; U_{in}, liquid velocity at the interface, m/sec; U_{∞}, liquid velocity at the outer edge of the boundary layer, m/sec; ΔU_{∞} , motive force of momentum transfer, m/sec; V_{∞} , velocity of the droplet motion, m/sec; y, transverse coordinate, m; δ , boundary layer thickness, m; ε , energy dissipation, m²/sec³; μ , dynamic viscosity, Pa·sec; $\mu^* = \mu_1/\mu_2$; ν , kinetic viscosity, m²/sec; ξ_d , ξ_s , resistance coefficients of the droplet and the sphere; σ , surface tension, N/m; τ , momentum flux, Pa; β , mass transfer coefficient, m/sec; γ , momentum transfer coefficient, m/sec; ρ , density, kg/m³. Complexes: Re_d = 2V_{∞}R_d/ ν , Reynolds number for the droplet; Sc = ν/D , Schmidt number; $R_{\delta} = U_*\delta/\nu$. Subscripts: 1, dispersed phase; 2, solid phase.

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