NOTATION

Here r is the microparticle radius; ρ, microparticle density; V, velocity; F_E, force due to electric field; q, charge; E, electric field strength; g, acceleration due to gravity; F_g, gravitational force; m, microparticle mass; F_c, drag force of medium; η, viscosity of medium; F_n, nonsteady term in equation of motion; s, drag force of medium per unit velocity; τ_p, time constant of particle; τ, time of free flight; q_M, maximum charge; ε, ε_0, dielectric permittivity; x, coordinate; f, distribution function; d, interelectrode distance; sign, sign function; δ, delta function; n, concentration; Φ, intensity of scattering flux; β, scattering cross section; t, time; h, norm; N_M, number of interparticle collisions; N_e, number of collisions with electrodes; N_0, total number of collision; $\tilde{n}$, scatterer concentration; $\tilde{V}$, relative velocity; l, free path length; $\mu_{0,S}$, chemical potential; $\varepsilon_{0,S}$, potential energy; U, potential difference; J, current density; γ, surface concentration.

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PULSATIONAL CHARACTERISTICS OF THE MODEL OF MASS FLOW IN A FLOW-THROUGH REACTOR

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Liquid flow in a flow-through reactor and one-dimensional longitudinal turbulent mass transfer is considered. The turbulent mass flux is described by a second-order differential equation including the velocity and spatial scale of the turbulent pulsations. Conditions of pulsed tracer introduction in the reactor are considered, and the inverse problem for experimental determination of the pulsational characteristics is solved by the moment method.

In [1, 2], an inhomogeneous differential equation was obtained for the isotropic one-dimensional turbulent or molecular mass (heat) transfer

$$l^2\frac{\partial^2 q}{\partial x^2} - \frac{l^2}{u^2}\frac{\partial^2 q}{\partial \tau^2} - \frac{2l}{u}\frac{\partial q}{\partial \tau} - q = ul\frac{\partial C}{\partial x}, \tag{1}$$

which includes the spatial scale l and velocity u of the pulsations.

The model in Eq. (1) differs from those in [3, 4] in that the spatial scale and second derivative of the flux with respect to the coordinate are individually present. This permits the formulation of a boundary problem for the flux q which more correctly reflects the physical picture at the boundaries (walls) of the reactor. The steady (quasi-steady at large u) model

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$$l^2 \frac{\partial^2 q}{\partial x^2} - q = ul \frac{\partial C}{\partial x} \tag{2}$$

like the model in Eq. (1) but in contrast to classical gradient laws, ensures finiteness of the flux at high values of the concentration gradients, and may be used to model processes with intense mass transfer or a high rate of chemical reaction [2].

The practical application of Eqs. (1) and (2) for modeling mass transfer in a specific type of reactor entails knowing numerical values of the parameters l and u and also their dependence on the operating conditions of the reactor (for example, on the rotation frequency of the mixing unit) and the physical properties of the medium. In the present work, a method of determining these parameters is considered for the case of a homogeneous flow-through reactor. The material-balance equation is

$$\frac{\partial C}{\partial \tau} = -u_x \frac{\partial C}{\partial x} - \frac{\partial q}{\partial x} \tag{3}$$

and the corresponding boundary condition at the reactor input is

$$C(0, \tau) = C_{in} \tag{4}$$

Consider the case most often encountered in practice, in which the walls at the reactor input and output are impermeable to the flux q. The boundary conditions for Eq. (1) are

$$q(0, \tau) = q(L, \tau) = 0. \tag{5}$$

Suppose that the tracer concentration in the reactor initially is zero, and that it is fed to the reactor input in pulsed fashion. In this case

$$C(x, 0) = 0; \quad C_{in} = \delta_+(\tau); \quad q(x, 0) = \frac{\partial q(x, 0)}{\partial \tau} = 0. \tag{6}$$

The conditions in Eq. (6) are typical in investigating the hydrodynamic structure in flow-through equipment [5]. Introducing the dimensionless variables and parameters $X = x/L$; $T = \tau/\bar{\tau} = u_x\tau/L/$ $C' = C/C^*$; $Q = q/uC^*$; $M = L/l$; $\delta = u_x/u$, Eqs. (1), (3), and (4)-(6) may be written in the form

$$\frac{\partial C'}{\partial T} = -\frac{1}{\delta} \frac{\partial Q}{\partial X} - \frac{\partial C'}{\partial X}; \tag{7}$$

$$\frac{\partial^2 Q}{\partial X^2} - \delta^2 \frac{\partial^2 Q}{\partial T^2} - 2\delta M \frac{\partial Q}{\partial T} - M^2 Q = M \frac{\partial C'}{\partial X}; \tag{8}$$

$$Q(0, T) = Q(1, T) = 0;$$

$$C'(0, T) = \frac{1}{\bar{\tau}} \delta_+(T); \quad C'(X, 0) = 0; \tag{9}$$

$$Q(X, 0) = \frac{\partial Q(X, 0)}{\partial T} = 0. \tag{10}$$

The variation in tracer concentration at a definite point of the reactor, for example, at the output, is measured experimentally, and the parameters M and δ may be found if the inverse problem is solved. For its solution, the following central moments are introduced

$$\mu_i(X) = \int_0^\infty C'(X, T)(T-1)^i \, dT; \tag{11}$$

$$Q_i(X) = \int_0^\infty Q(X, T)(T-1)^i \, dT \quad (i = 2, 3), \tag{12}$$

related to the dimensional moments

$$\mu_i^\tau(x) = \int_0^\infty C'(x, \tau)(\tau - \bar{\tau})^i\, d\tau; \tag{13}$$

$$Q_i^\tau(x) = \int_0^\infty Q(x, \tau)(\tau - \bar{\tau})^i\, d\tau \tag{14}$$

as follows

$$\mu_i^\tau = (\bar{\tau})^{i+1}\mu_i; \quad Q_i^\tau = (\bar{\tau})^{i+1} Q_i. \tag{15}$$

The mean residence time is

$$\bar{\tau} = \int_0^\infty C(L, \tau)\,\tau d\tau. \tag{16}$$

Applying the integral transformations in Eqs. (11) and (12) to the system in Eqs., (7)-(10), the following problem is obtained for finding μ_i and Q_i

$$\frac{d^2Q_i}{dX^2} + \frac{M}{\delta}\frac{dQ_i}{dX} - M^2Q_i = iM\mu_{i-1}(X) + i(i-1)\delta^2 Q_{i-2} - 2i\delta M Q_{i-1}; \tag{17}$$

$$\mu_i(X) = \frac{(-1)^i}{\bar{\tau}} - \frac{Q_i(X)}{\delta} + i\int_0^X \mu_{i-1}(X)\, dX; \tag{18}$$

$$Q_i(0) = Q_i(1) = 0. \tag{19}$$

For quasi-steady Eq. (2)

$$\frac{d^2Q_i}{dX^2} + \frac{M}{\delta}\frac{dQ_i}{dX} - M^2Q_i = iM\mu_{i-1}(X). \tag{20}$$

Omitting the cumbersome solution of Eqs. (17)-(20), the final expressions for the dimensionless central moments of second and third order calculated at the reactor output with $x = L$ are given here

$$\beta_2 = \frac{2}{M\delta} + \frac{2K\alpha}{(M\delta)^2}[1 - \exp(\lambda_1)]; \tag{21}$$

$$\beta_3 = \frac{6}{M^2\delta}\left[\frac{1}{\delta} + 2\Gamma(1 - \alpha + \alpha^2) - \frac{K(1-2\alpha)}{\delta}\right] + $$

$$+ \frac{6\alpha[1 - \exp(\lambda_1)]}{M}\left[\frac{K(\Gamma - M + 1/\delta)}{(M\delta)^2} + \frac{\Gamma(1-2\alpha)}{M\delta} + \right.$$
$$\left. + \frac{1}{\lambda_1^2}\left(\frac{1}{\delta} + \frac{\Gamma}{K}\right) - \frac{1}{\lambda_2^2}\left(\frac{1}{\delta} - \frac{\Gamma}{K}\right)\right]; \tag{22}$$

where

$$\lambda_1 = \frac{M}{2\delta}(K - 1); \quad \lambda_2 = -\frac{M}{2\delta}(K + 1);$$
$$K = \sqrt{1 + 4\delta^2}; \quad \alpha = \frac{1 - \exp(\lambda_2)}{\exp(\lambda_1) - \exp(\lambda_2)}; \tag{23}$$

$$\Gamma = \begin{cases} 1/\delta + 2\delta \text{ for the nonsteady model in Eq. (1),} \\ 1/\delta \text{ — for the quasi-steady model in Eq. (2);} \end{cases}$$
$$\beta_2 = \frac{\mu_2^\tau(L)}{(\bar{\tau})^2}; \quad \beta_3 = \frac{\mu_3^\tau(L)}{(\bar{\tau})^3}. \tag{24}$$

Note that the moments μ_0 and μ_1 calculated when $x = L$ do not give any information on the parameters M and δ. It is evident from Eq. (23) that, when $\delta < 0.1$ ($u \gg u_x$), Γ is practically independent of the choice of Eq. (1) or Eq. (2). This situation is characteristic for equipment with intense mechanical mixing, and in this case the use of the simpler Eq. (2) is justified.

When $\delta > 0.1$-0.2, the use of the quasi-steady model in the given nonsteady process is not justified. This is characteristic, for example, of the turbulent flow of liquid or gas in hollow reactors where $u \approx (0.1\text{-}0.2)u_x$. Equation (21) does not include Γ, i.e., the expression for the second moment does not depend on whether Eq. (1) or Eq. (2) is used. Generalizing the approach to obtaining Eqs. (21) and (22), it may be concluded that the moment β_2 is "insensitive" to the terms $(l^2/u^2)\partial^2 q/\partial\tau^2$ and $(2l/u)dq/\partial\tau$ in Eq. (1); the moment β_3 is "insensitive" to the term $(l^2/u^2)\partial^2 q/\partial\tau^2$; the fourth-order moment is "sensitive" to all the terms in Eq. (1).

Thus, the parameters δ and M may be determined using the two algebraic Eqs. (21) and (22), which may be solved numerically. Numerical values of β_2 and β_3 are obtained on the basis of the experimental differential distribution function $C(L, \tau)$ of the tracer residence time in the reactor and the application of numerical integration to Eqs. (13) and (16).

Note, in conclusion, that at large u ($\delta \to 0$) and finite M, it follows from Eqs. (21) and (22) that

$$\beta_2 \approx \frac{2}{M\delta} - \frac{2}{(M\delta)^2}[1 - \exp(-M\delta)];$$
$$\beta_3 \approx \frac{12[1 + \exp(-M\delta)]}{(M\delta)^2} - \frac{24[1 - \exp(-M\delta)]}{(M\delta)^3}. \tag{25}$$

If $M\delta = (L/l)(u_x/u) = u_x L/D$ is regarded as the Peclet number, Eq. (25) will coincide with the well-known equations for the diffusional model [5].

CONCLUSION

For the most widespread experimental method of investigating the hydrodynamic structure of the flow in flow-through reactors — i.e., the pulsed introduction of tracer at the reactor input and the recording of the differential distribution of the residence time (DFRT) — theoretical expressions are obtained for the second and third central moments of the DFRT within the framework of the model of turbulent mass flow described by the second-order Eq. (1), the parameters of which are the pulsation velocity and the spatial scale of the pulsations.

NOTATION

Here τ is time, sec; x, coordinate, m; C, C_{in}, current tracer concentration and concentration at the reactor input, kg/m^3; C^*, concentration scale, kg/m^3; u, mean pulsation rate, m/sec; l, spatial scale of pulsations, m; q, mass flux, kg/m^2·sec; L, reactor length, m; u_x, velocity of translational motion, m/sec.

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