length along flow axis; t, time; C, impurity concentration; D, coefficient of molecular diffusion; D_{ef}, effective-diffusion coefficient.

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MATHEMATICAL MODELING OF PARTICLE GROWTH

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Continuity equations for particle distributions by size and residence times are considered in processes associated with particle growth. The relation between these equations and the particle-balance equation in phase space is shown.

Particle-balance equations (continuity equations for particle distributions) occupy an important place in the study of processes associated with particle growth [1-11]. The most general approach to the formulation of such equations was outlined in [12, 13], which proposed the description of a heterogeneous process associated with any transformation of particles of a disperse phase, such as the motion of a point reflecting the state of the particle in a multidimensional phase space (a phase space is taken to be a system of spatial coordinates and coordinates characterizing the internal state of the particle). The particle-balance equation in this case is

$$\frac{\partial \rho_1}{\partial t} + \operatorname{div}(\vec{\omega}\rho_1) + \sum_{k=1}^{m} \frac{\partial}{\partial \xi_k}\left(\rho_1 \frac{d\xi_k}{dt}\right) = \psi_1, \tag{1}$$

where $\rho_1 = \rho_1(x, y, x, \xi_1, \ldots, \xi_m)$ is the density of the particle distribution.

For a nonideal system, terms characterizing particle mixing must be introduced in Eq. (1). For example, if particle mixing proceeds by the diffusion law, the appropriate equation is

$$\frac{\partial \rho_1}{\partial t} + \operatorname{div}(\vec{\omega}\rho_1 - D \operatorname{grad} \rho_1) - \sum_{k=1}^{m} \frac{\partial}{\partial \xi_k}\left(\rho_1 \frac{d\xi_k}{dt}\right) = \psi_1. \tag{2}$$

In processes of particle growth, the particle size serves as the internal coordinate. If growth is accompanied by other processes (drying, chemical change, etc.), coordinates characteristic for these processes (moisture content, degree of transformation, etc.) must be introduced into the equation. As a rule, however, all these parameters may be represented as different functions of a single variable — τ, the residence time of the particle in the apparatus. Thus, Eq. (2) may be written in the form

$$\frac{\partial \rho_2}{\partial t} + \operatorname{div}(\vec{\omega}\rho_2 - D \operatorname{grad} \rho_2) + \frac{\partial \rho_2}{\partial \tau} = \psi_2, \tag{3}$$

where $\rho_2 = \rho_2(x, y, z, \tau)$.

It can easily be shown that several known solutions of the balance equations in processes of particle growth [1-11] are partial cases of the solution of Eqs. (2) and (3) for conditions of ideal mixing and ideal substitution. In the present work, an attempt is made to solve the continuity equation of the particle distribution in the diffusion model for nonideal conditions.

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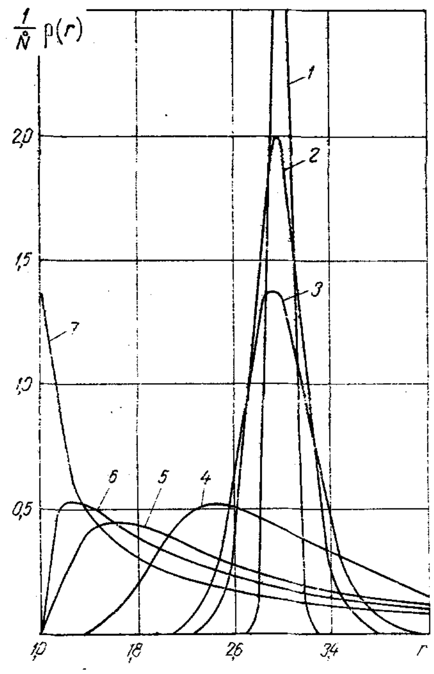

Fig. 1. Density of particle distribution by size for various values of $D_x/w_x l$ = 1/Pe (r_i = 1 mm; m_p = 3 mm): 1) 1/Pe = 0.0005; 2) 0.005; 3) 0.01; 4) 0.1; 5) 0.5; 6) 1; 7) 1/Pe = 5. $(1/\mathring{N})\rho(r)$, mm^{-1}; r, mm.

In the one-dimensional case, for steady conditions, and in the absence of particle sources of sinks (for w_x = const and w_p = const), Eqs. (2) and (3) take the form

$$w_p \frac{\partial \rho(r, x)}{\partial r} + w_x \frac{\partial \rho(r, x)}{\partial x} - D_x \frac{\partial^2 \rho(r, x)}{\partial x^2} = 0, \tag{4}$$

$$w_x \frac{\partial \rho(\tau, x)}{\partial x} - D_x \frac{\partial^2 \rho(\tau, x)}{\partial x^2} = 0. \tag{5}$$

In solving Eqs. (4) and (5), the following initial conditions are taken: $\tau = 0$; $x = 0$; $r = r_i$; $\rho(\tau, 0) = \mathring{N}\delta(\tau)$; and $\rho(r, 0) = \mathring{N}\delta(r - r_i)$. At the exit from the apparatus, $(x = l)$, the solutions are

$$\rho(r, l) = \frac{\mathring{N}}{2 w_p \tau_0 \sqrt{\pi \left(\frac{D_x}{w_x l}\right) w_p \tau_0 (r - r_i)}} \exp\left[-\frac{[w_p \tau_0 - (r - r_i)]}{4\left(\frac{D_x}{w_x l}\right) w_p \tau_0 (r - r_i)}\right], \tag{6}$$

$$\rho(\tau, l) = \frac{w_x \mathring{N}}{2\sqrt{\pi D_x \tau}} \exp\left[-\frac{(l - w_x \tau)^2}{4 D_x \pi}\right]. \tag{7}$$

As is evident from Fig. 1, the broadest spectrum of the particle distribution by size corresponds to ideal mixing ($D_x/w_x l \to \infty$) and the narrowest, to ideal substitution ($D_x/w_x l \to 0$). For initially monodisperse conditions, the latter case corresponds to a monodisperse product with particle size $r = r_i + w_p \tau_0$.

The characteristics of the particle distribution by size necessary to determine the parameters of the distribution from experimental data are the maximum density of the distribution

$$\rho_{max} = \frac{\mathring{N}}{2 w_p \tau_0 \sqrt{\pi \left(\frac{D_x}{w_x l}\right) \sqrt{\left(\frac{D_x}{w_x l}\right)^2 - \frac{D_x}{w_x l}}}} \exp\left[-\frac{\sqrt{\left(\frac{D_x}{w_x l}\right)^2 + 1} - 1}{2\left(\frac{D_x}{w_x l}\right)}\right], \tag{8}$$

the mode

$$r_{\text{M}} = w_{\text{p}}\tau_0 \left[\sqrt{\left(\frac{D_x}{w_x l}\right)^2 + 1} - \frac{D_x}{w_x l} \right] + r_{\text{i}}, \tag{9}$$

the mathematical expectation

$$m_{\text{p}} = w_{\text{p}}\tau_0 \left[2\left(\frac{D_x}{w_x l}\right) + 1 \right] + r_{\text{i}}, \tag{10}$$

and the dispersion

$$\sigma_{\text{p}}^2 = \left[8\left(\frac{D_x}{w_x l}\right)^2 + 2\left(\frac{D_x}{w_x l}\right) \right] (w_{\text{p}}\tau_0)^2. \tag{11}$$

This solution may be used to analyze processes associated with particle growth (dehydration of solutions, granulation of melts, etc.) occurring in apparatus of drum-granulator type — dryers, equipment with a fluidized bed of corrugated type, and a variety of other nonideal apparatus.

NOTATION

D, mixing coefficient; l, length of apparatus; $\overset{\circ}{N}$, number of particles in unit working volume of the apparatus; r, radius of the particle at any instant; r_i, initial radius of particle; t, time; $\vec{w}$, vector of particle velocity; w_p, particle growth rate; x, y, z, spatial coordinates of particle; $\delta(r-r_i)$, $\delta(\tau)$, delta functions; $\xi_1, \ldots, \xi_m$, internal coordinates of particle; ρ_1, ρ_2, densities of particle distribution (number of particles per unit volume of phase space); τ, residence time of particle in apparatus; τ_0, mean residence time; ψ_1, ψ_2, densities of particle sources and sinks.

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