THE CALCULATION OF PARTICLE TRAJECTORIES IN FLUIDIZED BED APPARATUS

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The problem arising in investigations of chlorination of polymers in a "boiling bed" was formulated in [1, 2]. It was found necessary to take into consideration the trajectories of particles and to introduce a certain special measure in the space of these trajectories. The method of solving this problem is presented together with the results of calculations for two separate variants.

We consider the process in which the random function describing one-dimensional particle motion in the apparatus satisfies the equation of unsteady convective diffusion

$$\frac{\partial F}{\partial t} = D_0 \frac{\partial^2 F}{\partial x^2} - w_0 \frac{\partial F}{\partial x} \tag{1}$$

with the following initial and boundary conditions:

$$F(0, x) = \begin{cases} 0 \text{ for } x < x_0, \\ 1 \text{ for } x \geqslant x_0; \end{cases}$$
$$F(t, 0) = 0, \quad \frac{\partial F}{\partial x}(t, H) = 0. \tag{1a}$$

The physical meaning of these equations is as follows: in the apparatus, local convective diffusion of the solid phase takes place at every point, and the particle displacement is determined, first, by a translation proportional to the solid-phase feed rate to the apparatus, and, secondly, by a random translation of a purely diffusional nature. Function $F(t, x, \tau, x_0)$ represents the probability that a particle, which at time τ is at point x_0, will be in the interval $[0, x]$ at time t. These are the so-called transitional probabilities of the process. The solution is sought in the interval [O, H], where H is the height of the apparatus. With time measured in units of H/w_0 and the coordinate x along the apparatus in units of H, the system of equations (1), (1a) becomes

$$\frac{\partial F}{\partial t} = D\frac{\partial^2 F}{\partial x^2} - \frac{\partial F}{\partial x}, \quad D = \frac{D_0}{Hw_0}; \tag{1'}$$

$$F(\tau, x) = \begin{cases} 1 & x \geqslant x_0, \\ 0 & x < x_0; \end{cases}$$

$$F(t, 0) = \frac{\partial F}{\partial x}(t, 1) = 0. \tag{1a'}$$

The solution of Eq. (1') with conditions (1a') is written in series form:

$$F(t, x, \tau, x_0) = 2\exp\left[\lambda(x - x_0)\right] \times$$
$$\times \sum_{n=1}^{\infty} \frac{\exp\left[(\mu_n^2 D + \mu)(t - \tau)\right](\lambda \sin \mu_n x + \mu_n \cos \mu_n x)}{(\lambda^2 + \mu_n^2)\left(1 - \frac{\sin 2\mu_n}{2\mu_n}\right)} \times$$
$$\times \sin \mu_n x. \tag{2}$$

Here $\lambda = 1/2D$, $\mu = -1/4D$, and μ_n satisfies the transcedental equation

$$\operatorname{ctg} \mu_n = -\frac{\lambda}{\mu_n}. \tag{3}$$

A particle of radius R moving along trajectory x(t) reacts with the surrounding gas containing, for example, chlorine, which diffuses into the particle, as defined by equation

$$\frac{\partial c_1}{\partial t} = D_1\left(\frac{\partial^2 c_1}{\partial r^2} + \frac{2}{r}\frac{\partial c_1}{\partial r}\right) - kc_1 \tag{4}$$

with initial and boundary conditions

$$c_1(r, 0) = 0, \quad \frac{\partial c_1}{\partial r}(0, t) = 0,$$
$$c_1(1, t) = \beta c^*\left[x(t)\right]. \tag{4a}$$

The diffused chlorine combines with the substance of the particle according to the equation

$$\frac{dc_2}{dt} = kc_1 \tag{5}$$

with initial condition

$$c_2(r, 0) = 0. \tag{5a}$$

Here the concentrations c_1, c_2, and c^* are expressed in units of c_0^*, r in units of R, and time t in units of H/w_0,

$$D_1 = \frac{DH}{w_0 R^2}, \quad k = \frac{k_0 H}{w_0}.$$

To solve Eqs. (4) and (5) it is necessary to know the particle trajectory.

Let us consider one of the methods of calculating the particle trajectory. We solve Eq. (1') with conditions (1a') and $\tau = 0$, $x_0 = 0$ in a sufficiently small interval of time Δt, selecting a random coordinate x_1 for the particle in accordance with the obtained distribution function. We then solve Eq. (1), (1a) in the interval Δt with condition $\tau = 0$, $x_0 = x_1$, and select coordinate x_2, and so on, continuing this process until $x_n \geq 1$ is obtained. The corresponding time $T = n\Delta t$ is the instant when the particle leaves the apparatus. In this manner we derive a sequence of points $x_1, x_2, \ldots, x_n$ which define the particle trajectory. We assume that between these points the motion of the particle is uniform. The smaller the selected intervals Δt, the more accurate the approximation to the true trajectory of the particle. Having determined the particle trajectory x(t), we can solve Eqs. (4) and (5). Two variants are of interest: A) the chlorine concentration $c^*(x)$ in the apparatus is maintained externally, and B) this concentration is maintained at the inlet to the apparatus.

A. For simplicity's sake let us consider the case in which $c^* = ax + b$. The mass $m_2([x], T, \tau)$ of bound chlorine in the particle introduced into the apparatus at time τ, moving along trajectory x(t) up to instant T (T is the time at which the particle leaves the apparatus along the trajectory x(t)) is

$$m_2 = 4\pi \int_0^1 c_2(r, T) r^2 dr.$$

The solution of Eq. (4) is of the form

$$c_1(r, t) = c^*[x(t)] + \sum_{n=1}^{\infty} u_n(t) \frac{\sin v_n r}{r}, \tag{6}$$

where

$$u_n = 2(-1)^n \left[\frac{c^*[x(t)]}{v_n} - v_n D_1 \exp(-A_n t) \times \right.$$
$$\left. \times \int_0^t \exp(A_n \tau) c^*[x(\tau)]\, d\tau \right];$$
$$v_n = \pi n; \quad A_n = k + v_n^2 D_1,$$

and, since

$$m_2 = 4\pi k \int_0^T \int_0^1 c_1(r, \tau) r^2 dr d\tau. \tag{7}$$

Substituting (6) into (7) and taking into account that $c^* = ax + b$ and that for $t \in \Delta t$, x(t) is a piecewise linear function of the form $x_i + ((t - t_i)/\Delta t)(x_{i+1} - x_i)$ we obtain (omitting the cumbersome intermediate calculations)

$$m_2 = 8\pi D_1 k \left\{ b \sum_{n=1}^{\infty} \frac{A_n T + \varphi(T) - 1}{A_n^2} + \right.$$
$$+ a \sum_{n=1}^{\infty} \frac{1}{A_n^2} (1 + \varphi(\Delta t) - A_n \Delta t) \times$$
$$\left. \times \left(\frac{1}{2} + \sum_{s=1}^{M-1} E_s + P \sum_{s=1}^{M-2} (B_s - N_s) + \frac{x_{M-1}}{2} \right) \right\},$$

$$\varphi(x) = \exp(-A_n x); \quad B_s = x_s \frac{1 - \varphi[\Delta t(M - s)]}{1 - \varphi(\Delta t)};$$

$$E_s = x_s \frac{1 - \varphi[\Delta t(M - s + 1)]}{1 - \varphi(-\Delta t)} - \frac{x_s}{2} \varphi[\Delta t(M - s)];$$

$$P = [1 - \varphi(\Delta t) - A_n \Delta t \varphi(\Delta t)];$$

$$N_s = \frac{x_s}{2} \varphi[\Delta t(M - s - 1)].$$

Here $M = T/\Delta t$. Having determined a sufficient number of trajectories, we can obtain the distribution of the chlorine content in the outgoing product.

B. In practice this is the more important case, since it is difficult to sustain in the apparatus a specified concentration profile of the reactive gas.

An examination of the material balance of an element of the apparatus volume (on condition of ideal displacement by the gaseous phase) yields for the chlorine concentration $c^*(x)$ in the gaseous phase the equation

$$w_1 \frac{dc^*}{dx} = D_0 \left[\frac{d\bar{m}}{dx} \frac{dc}{dx} + \right.$$
$$\left. + \bar{m}(x) \frac{d^2c}{dx^2} \right] + w_0 c \frac{d\bar{m}}{dx}. \tag{8}$$

Here c is the concentration of particles in the apparatus, and $\bar{m}(x)$ is the mean chlorine content (bound and free) in a particle in section x of the apparatus. The expression for $\bar{m}(x)$ can be derived as follows: we denote by $m([x], t, \tau)$ the mass of the bound and the free chlorine in a particle entering the apparatus at time τ and moving along trajectory x(t) up to time t. Since a stationary process is considered here, the trajectories of particles introduced at time τ_1 lag with respect to those introduced at time τ by $\tau_1 - \tau$, i.e.,

$$m([x], t, \tau) = m([x], t - \tau).$$

Let us now consider only those of the particles which had entered the apparatus at time $\tau < t$, and which at time t are in section y of the appratus. The average chlorine content in such particles is

$$\bar{m}(y, t - \tau) = \int_{[x]} m([x], t - \tau)\, d\mu_y,$$

where integration is carried out over all trajectories of particles entering the apparatus at time τ, and such that $x(t) = y$. At time t section y of the apparatus contains all of the particles introduced into it up to time t. If the feed rate of the solid phase into the apparatus is n, and the distribution density of the τ-particles in it at time t is $f(y, t - \tau)$, then the average amount of chlorine in particles occupying section y of the apparatus at time t is

$$\bar{m}(y) = \frac{\int_0^{\infty} n\bar{m}(y, t) f(y, t)\, dt}{\int_0^{\infty} nf(y, t)\, dt}.$$

It can be shown that in our case c = const, hence Eq. (8) becomes

$$\frac{dc^*}{dx} = \frac{n}{w_1} \frac{d\bar{m}}{dx}. \tag{9}$$

If g is the mass feed rate of the solid phase through a unit cross section of the apparatus, then $n = 3g/4\pi R^3\gamma$ is the number of particles entering the apparatus per unit of time. Selecting H, R, n, m_0, H/w_0, and c_0^* as the fundamental unit, we transform Eq. (8) into

$$\frac{dc^*}{dx} = QD \left[\frac{d^2c}{dx^2} \bar{m}(x) + \frac{dc}{dx} \frac{d\bar{m}}{dx} \right] + Qc \frac{d\bar{m}}{dx},$$

where $Q = m_0 n/w_1 c_0^*$ and $D = D_0/w_0 H$ are dimensionless complexes, and, correspondingly, Eq. (9) becomes

$$\frac{dc^*}{dx} = Q \frac{d\bar{m}}{dx}. \tag{9'}$$

Solving Eq. (9') we obtain

$$c^* = 1 + Q\bar{m}(x),$$

since $\overline{m}(0) = 0$, which corresponds to the physical meaning of function $\overline{m}(x)$. We assume here that $\overline{m}(x) = m([\overline{x}], t)$, where x(t) is the mean trajectory of particles, i.e.,

$$\bar{x}(t) = \int_0^1 xf(x, t)\,dx.$$

This assumption means in particular that the average chlorine content in particles in section y of the apparatus is equal to the chlorine content of a particle on trajectory $\overline{x}(t)$ at that time τ at which that particle finds itself in section y, i.e., when $\overline{x}(\tau) = y$. We can now write the expression for $c^*(x)$. Since the chlorine content in a particle on trajectory x(t) up to time t is $m([x], t)$, then $m_1([x], t)$ and $m_2([x], t)$ are, respectively, the contents of free and bound chloride in the particle moving on trajectory x(t) up to instant of time t and are given by

$$m_1 = 4\pi \int_0^1 c_1(r, t)\, r^2 dr,$$

$$m_2 = 4\pi k \int_0^1 \int_0^t c_1(r, t)\, r^2 dr$$

and $m = m_1 + m_2$. Substituting for $c_1(r, t)$ the corresponding expression (6), after lengthy calculations we obtain

$$c^*(x) = 1 + 8\pi Q \sum_{n=1}^{\infty} \left(\varphi_n(t) \int_0^t \varphi_n(-\tau)\, c^*[\bar{x}(\tau)]\, d\tau + k \int_0^t \varphi_n(s) \int_0^s \varphi_n(-\tau)\, c^*[\bar{x}(\tau)]\, d\tau\, ds \right),$$

$$\varphi_n(t) = \exp(-A_n t),$$

which is an integral Volterra equation. Its solution may be obtained by the method of successive approximations, with $c^*(x)$ expressed in terms of c_0^* [3].

We have thus obtained the expression for $c^*(x)$, and can now proceed with the calculation of $m_2([x], T)$ for our case. We cite certain of the estimates used in the summation of series expansions appearing in various formulas. Let us estimate the number of terms of expansion (2) required for calculating $F(\tau, x_0, t, x)$ with a specified accuracy.

Let R_N be the absolute value of the remainder of expansion (2). Since $(2n - 1) \cdot \pi/2 < \mu_n < \pi n$,

$$\left(1 - \frac{\sin 2\mu_n}{2\mu_n}\right) > \frac{1}{2},$$

$$\lambda^2 + \mu_n^2 > \mu_n^2, \quad |\sin \mu_n x| \leqslant 1.$$

Hence

$$R_N < \sum_{n=N}^{\infty} \frac{\exp(-\mu_n^2 c)(\lambda + \mu_n)}{\mu_n^2},$$

where $c = D(t - \tau)$.

The number R of terms of the expansion required for a specified accuracy of the calculation of $F(\tau, x_0, t, x)$ can be determined from the condition $R_N < \varepsilon$.

We used the following method for calculating $F(\tau, x_0, t, x)$. Function $F(\tau, x_0, t, x)$ is a monotonically increasing one, whose derivative has for small $(t - \tau)$ the following singularities: in the neighborhood of point x_0 we find $F' \gg 1$, while at some distance from that point $F' \ll 1$. Because of this $F(\tau, x_0, t, x)$ was calculated only in the neighborhood of point x_0. Away from point x_0 $F(\tau, x_0, t, x)$ was assumed to be equal to its value at point x at which calculations were still possible.

The mean trajectory was calculated as the arithmetic mean of a sufficient number of computed trajectories. Estimates of other expansions were derived in a manner similar to that used for expansion (2).

NOTATION

c(x) is the concentration of particles in a unit of the apparatus volume in section x; t is the time; H is the height of the apparatus; r is the coordinate along the radius of a particle; $c_1(r, t)$ is the concentration of free chlorine in a particle; $c^*(x)$ is the chlorine concentration in the apparatus; $m_1([x], t)$ is the total mass of free chlorine in a particle; $m_2([x], t)$ is the total mass of bound chlorine in a particle; w_0 is the linear velocity of a particle; q is the mass flow rate of particles through a unit section of the apparatus; D_0 is the coefficient of particle intermixing; w_1 is the gas linear velocity; D is the coefficient of gas diffusion in a particle; m_0 is the amount of chlorine to be absorbed by one particle; γ is the specific weight of the polymer; k_0 is the constant of the chemical reaction rate; c_0^* is the concentration of chlorine in the gas at the apparatus outlet.

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