IMPURITY DISPERSION IN CIRCULAR TUBE

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In describing various mass-transfer processes, wide use has been made of a diffusional model with an effective diffusion (dispersion) coefficient. The basic theory of dispersion was developed in [1, 2], where an equation with constant coefficients for the mean (over the cross section) particle concentration was proposed, together with a complex diffusion equation with a transfer rate depending on the coordinate transverse to the flow. Taylor calculated the dispersion coefficient and performed an experiment confirming the adequacy of the model. Subsequently, the dispersion theory was intensively developed, and several basic approaches to the derivation of the equivalent-diffusion equation and its generalization may be distinguished [3-5]. Here the dispersion equation is obtained by the small-perturbation method [6, 7], using Taylor considerations regarding the order of magnitude of terms in the initial diffusion equation. First, the impurity-dispersion equation is found with a weak dependence of the flow velocity on the impurity concentration. Then the problem is formulated for the first correction to the solution of the Taylor dispersion equation in the case of a parabolic profile of the flow velocity in the circular tube. Next, the analysis of the limiting solution of a characteristic nonsteady problem of impurity transfer around the wall of a prismatic channel of sufficiently general form is briefly considered.

The mass-transfer equation for the impurity is written in a coordinate system moving at velocity $\langle U\rangle = 2\int_0^1 rU(r)\,dr$ in the form ($v = U(r) - \langle U\rangle$)

$$\varepsilon^2 \frac{\partial c}{\partial t} + \varepsilon \frac{\partial}{\partial x}\{[v(r) + \varepsilon w(c,\ r)]\,c\} = \frac{1}{r}\frac{\partial}{\partial r}\left(r\frac{\partial c}{\partial r}\right), \tag{1}$$

where the dimensionless variables are related to dimensional equivalents as follows

$$\varepsilon = a^2u/DL,\quad t = \tau a^2u^2/DL^2. \tag{2}$$

The length scale L in the z direction is determined from the character of variation in the specified initial concentration

$$c|_{t=0} = F(x,\ r),\quad -\infty < x < +\infty. \tag{3}$$

It is assumed that $\underline{a} \ll L$, and so the term $\partial^2 c/\partial x^2$ is omitted in Eq. (1). Taking this term into account and other possible complications of the theory will be discussed below.

The boundary conditions for Eq. (1) are taken in the form

$$\partial c/\partial r|_{r=1} = 0,\quad c|_{r\to 0} \to \text{bounded}. \tag{4}$$

Assuming that ε is a small parameter, essentially the procedure of [1] is followed; in [1], the terms of an equation of the form in Eq. (1) were taken into account successively, on the basis of semiintuitive considerations, in the same order as will be adopted here when using the perturbation method. The velocity profile in Eq. (1) in the first approximation in ε takes account of the dependence of the velocity on the impurity concentration. Suppose that, with variation in concentration, the velocity rapidly relaxes to its equilibrium value. The functions U and w are assumed to be arbitrary, and the function F(x, r) is differentiable with respect to x.

Since ε is small, it is natural to seek the solution of the problem in Eqs. (1)-(4) in the form of an expansion

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$$c = c_0 + \varepsilon c_1 + \varepsilon^2 c_2 + \ldots, \tag{5}$$

and then substitution into Eq. (1) and grouping terms of the same order in ε gives the following equations

$$\partial (r \partial c_0/\partial r)/\partial r = 0, \tag{6}$$

$$\partial (r \partial c_1/\partial r)/\partial r = r v(r)\, \partial c_0/\partial x, \tag{7}$$

$$\partial (r \partial c_2/\partial r)/\partial r = r \partial\, [v c_1 + w(c_0,\ r)\, c_0]/\partial x + r \partial c_0/\partial t. \tag{8}$$

The boundary conditions for all the approximations will coincide with Eq. (4). Equations (6)-(8) may be solved successively. Note that these equations do not include time derivatives of the desired functions. Therefore, they describe the solution of Eqs. (1)-(4) only at sufficiently large times (external solution) [6].

Taking account of Eq. (4), Eq. (6) gives $c_0 = c_0(x,\ t)$. Then Eq. (7) has the solution

$$c_1 = c_1^0(x,\ t) + \frac{\partial c_0}{\partial x} \int_0^r \frac{dz}{z} \int_1^z \xi v(\xi)\, d\xi. \tag{9}$$

The equation for determining c_0 is obtained by integrating Eq. (8) with respect to r within the limits (0, 1), taking account of Eq. (9)

$$\frac{\partial c_0}{\partial t} + 2 \frac{\partial}{\partial x} \left\{ c_0 \int_0^1 r w(c_0,\ r)\, dr \right\} = D_0 \frac{\partial^2 c_0}{\partial x^2}, \tag{10}$$

where

$$D_0 = 2 \int_0^1 \frac{dr}{r} \left[\int_r^1 \xi v(\xi)\, d\xi \right]^2. \tag{11}$$

The dispersion coefficient D_0 was found earlier in [8] in somewhat more general form, taking account of the dependence of D on r. In the particular case when $w \equiv 0$ and with a parabolic velocity profile, Eq. (10) reduces to the Taylor equation [1]. Proceeding analogously, the equation for $c_1^0(x,\ t)$ may be found, etc. Below, the equation for $c_1^0(x,\ t)$ is found with a parabolic velocity profile, in the absence of nonlinear effects.

The initial condition for Eq. (10) may be obtained using the procedure of matching its solution with the solution of the internal problem. To this end, the internal time $T = t/\varepsilon^2$ is introduced, and an expansion of the type in Eq. (5) is taken for the internal problem

$$c = f_0(x,\ r,\ T) + \varepsilon f_1(x,\ r,\ T) + \ldots \tag{12}$$

It is simple to establish that the function f_0 satisfies the usual heat-conduction equation, and its asymptote as $T \to \infty$ takes the form

$$f_0(x,\ r,\ T) \underset{T\to\infty}{\sim} 2 \int_0^1 r F(x,\ r)\, dr \underset{t\to 0}{\sim} c_0(x,\ t), \tag{13}$$

where the latter relation is the principle of limiting matching [7] and Eq. (13) actually establishes the initial condition for Eq. (10)

$$c_0 |_{t=0} = 2 \int_0^1 r F(x,\ r)\, dr.$$

Note that the theory here outlined may be generalized, taking account of the chemical reaction both at the channel wall and in the flow volume. If the source term $\varepsilon^2 Q(c)$ is present in Eq. (1) and the boundary condition in Eq. (4) takes the form $\partial c/\partial r|_{r=1} = \varepsilon^2 q(c)$, then two terms $Q(c_0) + q(c_0)$ must be added to the right-hand side of Eq. (10). In the literature, doubts are expressed regarding the possibility of transferring the Taylor model to processes in the presence of chemical reaction [5, 9], since the basis of Taylor theory assumes no source terms in the equation. It is evident here that source terms may validly be introduced into the effective-diffusion equation if they are sufficiently small (of the order of ε^2). This agrees with the results of [9], where two solutions in the presence of a first-order reaction were compared: the solution of the Taylor model with the addition of a source; and the numerical solution of an equation of the type of Eq. (1). It was found that with decrease in intensity of the reaction (the factor preceding c) the difference in the results diminished. Note that the often-encountered case of a first-order reaction $Q = kc/\varepsilon^2$ may be accommodated within the Taylor scheme by means of the substitution $c = B\exp(-tk/\varepsilon^2)$. Then, for the new unknown function B, Eq. (1) is obtained without a source, i.e., the above procedure may be employed, reaching Eq. (10) for the variable B. According to the second formula in Eq. (2), the time scale at which the dispersion Eq. (10) operates is $DL^2/u^2\underline{a}^2$. At times of this order, i.e., $t = O(1)$, the function c is very small when $k = O(1)$, because of the exponential factor $\exp(-tk/\varepsilon^2)$ $(\varepsilon \to 0)$, so that the process is actually complete before dispersion effects appear. If $k = O(\varepsilon^2)$, the exponent is of the order of unity, and the chemical reaction is well described in the dispersion equations in accordance with the foregoing remarks.

If the term $\partial^2 c/\partial x^2$ is retained in Eq. (1), it will be preceded by the factor ε/Pe, where $\mathrm{Pe} = uL/D$. When $\mathrm{Pe} = O(1/\varepsilon)$, the above procedure leads to the formula of [3] for the dispersion coefficient. If $\mathrm{Pe} = O(1)$, however, difficulties in satisfying Eq. (4) arise in realizing the given algorithm. This is associated with the inexpedient choice of the order of terms in Eq. (1) in the given conditions. A more "compressed" time $\zeta = t/\varepsilon$ must be introduced. Then the procedure leads to the equation

$$\partial c_0/\partial\zeta = (1/\mathrm{Pe})\,\partial^2 c_0/\partial x^2 \tag{14}$$

for the zero-approximation function. Equation (14) may be used for smaller times than Eq. (10). In particular, as $\mathrm{Pe} \to \infty$, the result obtained is $\partial c_0/\partial\zeta = 0$, i.e., the usual transfer equation with velocity $\langle U\rangle$. This is the simplest case of the hyperbolic equations, which are encountered in describing dispersion phenomena [4, 5]. Equation (14) is "internal" (in the well-known sense) with respect to Eq. (1). On passing to the larger time scale t, it must agree with Eq. (1). However, it is evident that in Eq. (14) both terms are of the same order. Therefore, as $\zeta \to \infty$, i.e., on passing to Eq. (1), the terms $\partial c/\partial\tau$ and $D\partial^2 c/\partial z^2$ must be of the same order. Physically, this is explained in that as $\zeta \to \infty$, before dispersional effects of inhomogeneity of the velocity profile are felt, sufficiently strong "spreading" of the initial impurity-concentration distribution occurs because of molecular diffusion when $\mathrm{Pe} = O(1)$, and the choice of L as the length scale at such times ceases to be correct. These considerations agree with the results of [3], which showed that the molecular-diffusion coefficient must be added to the Taylor formula for the dispersion coefficient, without any constraints on Pe.

Equation (10) permits solutions in the form of a stationary wave $c_0 = c_0(\xi)$, $\xi = x - U_* t$. The first integral of Eq. (10) is

$$2c_0(\xi)\int_0^1 rw\,[c_0(\xi),\ r]\,dr = U_* c_0(\xi) + D_0\frac{dc_0}{d\xi} + A, \tag{15}$$

where A is a constant. This constant and the unknown wave velocity U_* must be determined using the boundary conditions at $\pm\infty$. If w may be represented by the following series, which is uniformly converging when $r \in [0, 1]$

$$w = \sum_{k=0}^{\infty} c_0^k \Omega_k(r), \tag{16}$$

then Eq. (10) takes the form of the equation

$$\frac{\partial c_0}{\partial t} + \frac{\partial\theta(c_0)}{\partial x} = D_0\frac{\partial^2 c_0}{\partial x^2}, \quad \theta(c_0) = 2\sum_{k=0}^{\infty} c_0^{k+1}\int_0^1 r\Omega_k(r)\,dr, \tag{17}$$

which appears in describing dissipation effects in nonlinear waves [10]. The integral in Eq. (15) changes correspondingly, after which c_0 is determined from Eq. (15) by simple quadrature. Note that often only the first two terms in the series in Eq. (16) need be considered in analysis; this corresponds to a weak impurity concentration. This case, is realized, for example, in describing the velocity profile in a tube by the Poiseuille formula with an effective value of the viscosity which is linearly dependent on the concentration in the first approximation. The corresponding coefficients in the expansion of w may be found, for example, from the Einstein formula [11] for the viscosity of suspensions. Linearizing Eq. (16) and passing to a coordinate system moving at velocity $2\int_0^1 r\Omega_0(r)\,dr$ in Eq. (17) – remember that Eq. (17) itself is written for a coordinate system moving at velocity <U> – leads to the Bürgers equation, which may be reduced to a heat-conduction equation, thereby significantly simplifying the analysis. Evidently, the Bürgers equation may be recommended for the description of nonlinear effects in impurity propagation in tubes, linearizing Eq. (16). Note the particular case $\int_0^1 rw(c_0, r)\,dr \equiv 0$, when Eq. (10) coincides with the Taylor equation and there are no nonlinear effects in the first approximation. Note also that the seemingly somewhat artificial definition of the order of the dependence of the flow velocity on the impurity concentration in Eq. (1) is justified in that, in the evolution of impurity transfer in a tube, nonlinear effects – no matter how small they may be initially – exert an influence at sufficiently large times, as in the analysis of nonlinear waves [10].

The expansion in Eq. (5) is refined to terms of order ε for the example when a Poiseuille velocity profile is realized in the tube ($v = 0.5 - r^2$), and w is zero. The function c_1 is expressed in terms of c_1^0 using Eq. (9); therefore, the problem is to find the equation which determines the function $c_1^0(x, t)$. It is obtained analogously to Eq. (10)

$$(1/192)\,\partial^2 c_1^0/\partial x^2 - \partial c_1^0/\partial t = (1/240)\partial^2 c_0/\partial x \partial t. \tag{18}$$

Dispersion theory is based on the mean concentration of material over the cross section, which is given by the expression

$$\langle c \rangle = 2\int_0^1 rc\,dr = c_0(x,\ t) + \varepsilon\,[c_1^0(x,\ t) + (1/24)\,\partial c_0/\partial x] + \ldots \tag{19}$$

Obtaining the initial condition in Eq. (18) only requires asymptotic (as T → ∞) information on the behavior of the solutions f_0 and f_1. As already noted, the function f_0 satisfies the heat-conduction equation. The equation for f_1 is

$$\partial f_1/\partial T + (0{,}5 - r^2)\,\partial f_0/\partial x = (1/r)\,\partial(r\partial f_1/\partial r)/\partial r, \tag{20}$$

i.e., the same heat-conduction equation but with a source term. These equations are subjected to Laplace transformation, and it is taken into account that [12]

$$\lim_{T\to\infty} g(T) = \lim_{p\to 0} pg^*(p). \tag{21}$$

Here and below, an asterisk denotes Laplace transformation of the quantity; p is the Laplace-transformation variable. To calculate the limit, the expansions of f_0^* and f_1^* in the vicinity of the point p = 0 must be obtained. The equation for f_0^* is

$$(1/r)\,d(rdf_0^*/dr)/dr = pf_0^* - F(x,\ r), \tag{22}$$

and it is simple to confirm that the desired expansion takes the form

$$f_0^* = \frac{2}{p}\int_0^1 rF(x,\ r)\,dr + \frac{r^2}{2}\int_0^1 rF(x,\ r)\,dr - \int_0^r \frac{dy}{y}\int_0^y \xi F(x,\ \xi)\,d\xi + R(x) + O(p), \tag{23}$$

where R(x) is some function of x which is not needed here. Using Eq. (23), the following asymptotic formula may be obtained from the Laplace-transformed Eq. (20)

$$f_1^* = \frac{2}{p}\left\{\left[\frac{r^2}{8} - \frac{r^4}{16}\right]\int_0^1 \xi F'_x(x,\ \xi)\,d\xi + \frac{1}{24}\int_0^1 rF'_x(x,\ r)(6r^2 - 3r^4 - 4)\,dr\right\} + O(1). \tag{24}$$

Now Eq. (5) is rewritten in internal variables, expanded in series in terms of ε, and Laplace-transformed. It is found that

$$c^* = \frac{c_0(x,\ 0)}{p} + \varepsilon\,\frac{c_1(x,\ r,\ 0)}{p} + \varepsilon^2\left[\frac{c_2(x,\ r,\ 0)}{p} + \frac{1}{p^2}\,\frac{\partial c_0}{\partial t}\bigg|_{t=0}\right] + \ldots \tag{25}$$

Taking account of Eq. (9), comparison of Eqs. (25), (23), and (24) gives the desired initial condition for Eq. (18)

$$c_1^0|_{t=0} = \frac{1}{24}\int_0^1 rF'_x(x,\ r)(6r^2 - 3r^4 - 4)\,dr. \tag{26}$$

Incidentally, the initial condition for Eq. (10) is obtained a second time. No fundamental difficulties appear either in obtaining the initial condition on an equation of the type in Eq. (18) or in the general case $w \not\equiv 0$ with any function v.

On the basis of the small-perturbation method, it is natural to suppose that the derivation of dispersion Eq. (10) and so on is only valid at small ε. Nevertheless, dispersion equations have been obtained previously by other methods [1-5] without isolating any small parameter and it is generally assumed that dispersion theory is applicable at sufficiently large times. This permits the hope that the approach here outlined may give equations that are also applicable when ε is not small.

It is interesting to consider the situation when $Pe_* = u\underline{a}/D \to \infty$, when ε need not be small. In this case, the central part of the channel rapidly becomes free of impurity on account of convective transfer. At the same time, the impurity will be present in a thin wall layer, where the transfer rate tends to zero, and will be fairly slow to leave the channel. Suppose that the channel walls do not have points where the radius of curvature of the contour is too large. For a channel of general form, it is convenient to proceed in s, n coordinates [13]. The limiting steady equation which is of interest here is obtained from the general convective-diffusion equation after the following deformation of the coordinates

$$\nu = T/\mathrm{Pe}_*^{1/3},\ N = n\,\mathrm{Pe}_*^{1/3} \tag{27}$$

and passing to the limit $Pe_* \to \infty$. Here n is measured from the channel surface. After appropriate computations, the desired boundary-layer equation is obtained

$$\partial c/\partial\nu + \beta(s)\,N\partial c/\partial z = \partial^2 c/\partial N^2 \tag{28}$$

where $\beta(s)$ depends on the form of the channel boundary and determines the slope of the velocity profile to the channel axis at boundary points. The coordinate s is "passive" in character (there is no differentiation with respect to s) in Eq. (28). This allows Eq. (28) to be brought to the following form by means of the variable substitution $Z = z/\beta(s)$

$$\partial c/\partial\nu + N\partial c/\partial Z = \partial^2 c/\partial N^2, \tag{29}$$

this equation is obtained in the analysis of the analogous problem in a circular tube [14], where Eq. (29) is solved with the following additional conditions

$$c|_{Z=0} = 0,\ c|_{\nu=0} = 1,\ \partial c/\partial N|_{N=0} = 0,\ c|_{N\to\infty} \to \text{bounded}, \tag{30}$$

corresponding to the problem of impurity extraction from the wall region of the channel. Using the results of [14], the following expression is obtained for $M = \int_0^\infty c\,dN$

$$M = \sum_{n=1}^{\infty} L_n K(Z,\ \nu\gamma_n),\ L_n = \left[\int_{-\gamma_n}^{\infty} \mathrm{Ai}(\xi)\,d\xi\right]^2 / \gamma_n \mathrm{Ai}^2(-\gamma_n), \tag{31}$$

where $\mathrm{Ai}(\xi)$ is the Airy function [15]; γ_n are the roots of the equation $\mathrm{Ai}'(-\gamma) = 0$, n = 1, 2, ..., and the following expansion exists for K

$$K(x,\ y) = \sqrt[3]{x}\sum_{n=0}^{\infty} \frac{(-1)^n}{n!\Gamma(4/3 - 2n/3)}\left(\frac{y}{x^{2/3}}\right)^n \sim \frac{27x^2}{8y^2\sqrt{\pi y}}\exp\left[-\frac{4y^3}{27x^2}\right], \tag{32}$$

where the first series is always convergent and the second is an asymptotic formula as $y/x^{2/3} \to \infty$. The information on the Airy function and the roots of its derivative required for the calculations may be found in [15]. The total amount of impurity in the channel is found by integrating Eq. (31) along the whole contour

$$\Phi = \sum_{n=1}^{\infty} L_n \int_0^l K\,[z/\beta(s),\ \nu\gamma_n]\,ds. \tag{33}$$

Equation (32) shows that M and Φ actually depend on the self-similar variable $\nu/z^{2/3}$. When this variable is large, the Laplace method [12] may be used to calculate the integrals in Eq. (33), and also the sums in Eqs. (31)-(33) may be limited to a single term. Substitution of the numerical values of the coefficients L_1 etc. [15] gives the expression

$$\Phi \sim \frac{18{,}1 z^3}{\nu^4 \beta^{5/2}(s_0)[\beta''(s_0)]^{1/2}} \exp\left[-\frac{0{,}1567\nu^3\beta^2(s_0)}{z^2}\right] \tag{34}$$

under the conditions that $\beta(s)$ permits the application of the Laplace method to the integrals in Eq. (33), and the asymptotic behavior of these integrals is determined solely by a single stationary point s_0 (the generalization to several stationary points is obvious). In addition, $\beta(s)$ is assumed to satisfy the inequality $\beta(s) \geq \beta_* > 0$. Physically, Eq. (34) means that, at sufficiently large times, the basic quantity of impurity in the channel will be concentrated at the point of the channel generatrix where the transfer conditions are worst, more precisely, where the velocity profile has the smallest inclination to the channel axis. Thus, only the transfer-rate characteristics at the wall at the point with the smallest inclination of the velocity profile to the channel contour are significant in considering the asymptotic pattern of impurity extraction from the channel.

NOTATION

a, tube radius; c, impurity concentration; D, molecular diffusion coefficient; D_0, dispersion coefficient (dimensionless); Pe = uL/D, Pe_* = ua/D, Peclet numbers; ℓ, length of channel contour; Q, q, intensity of chemical conversion of material (volume and surface rates, respectively); r, dimensionless (referred to a) radial coordinate; u, maximum flow velocity in tube; U_*, wave velocity; U(r), basic part of velocity in channel; <U>, mean velocity; v = U(r) − <U>; w, velocity perturbation, depending on impurity concentration; x = z/L; z, dimensional coordinate along channel; $\zeta = t/\varepsilon$; $\theta(c)$, as defined in Eq. (17); $\xi = x - U_* t$, self-similar variable; Φ, impurity volume in channel; $\Gamma(z)$, Euler gamma function; τ, time; Ω_k, functions in the expansion of w, Eq. (16).

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