

DISPERSION OF DYNAMICALLY PASSIVE IMPURITIES IN NON-ONE-DIMENSIONAL LIQUID FLOW

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Equations that describe dispersion of a substance in a non-one-dimensional incompressible liquid flow through a plane channel are derived. The model under consideration extends the traditional Taylor model to the case where sources of the substance are present in the flow and relaxation transfer processes are taken into account. Additional conditions for the dispersion equations are obtained. The relation between the proposed model and the Taylor model is analyzed. Based on the equations obtained, the mass transfer between circulation regions in the flow is calculated and a system of cellular-model equations for stagnant cavities is constructed.

Key words: dispersion of substance, diffusion (Taylor) model, wave model, heat and mass transfer, relaxation phenomena.

Introduction. The Taylor model of longitudinal dispersion of the substance has found wide application in predicting heat- and mass-transfer processes [1]. This model is based on the effective-diffusion (dispersion) equation that contains one variable less as compared to the master equation of convective diffusion. In fact, the Taylor model is an asymptotically substantiated (under certain conditions) averaging of the convective-diffusion equation. Unlike the initial equation of convective diffusion, the dispersion equation for one-dimensional flows through pipes of various configurations contains only constant coefficients. This simplification (in view of the broad range of its practical applications) has aroused considerable interest in the Taylor model, finally resulting in generalization of this model to the case of more complex heat- and mass-transfer phenomena; in this way, many novel approaches to the derivation of dispersion equations for a substance have been invented (see, for instance, [2–4]).

Yet, the dispersion equation, as an approximation to the master equation of convective diffusion, has a limited area of applicability, is incapable of providing required calculation accuracy, and allows no qualitative analysis of such problems to be performed. The shortcomings of the Taylor model were discussed in many publications (see, e.g., [5, 6]). The main drawback of the Taylor model is its inapplicability to problems with intense heat and mass sources. Since the Taylor diffusion model forms the basis for analyzing chemical flow reactors, where an increased rate of chemical transformations is often desirable, the mentioned drawback is obviously essential. That is why more general models for relaxation and wave phenomena under the presence of heat and mass fluxes were developed [5–7]. In the present paper, this model is considered in the general form. Calculations by the proposed model enable one to solve heat- and mass-transfer problems for non-one-dimensional flows (e.g., for flows in caverns).

1. Derivation of Basic Equations. We consider a plane problem. The mass transfer in a channel of height h is governed by the equation of convective diffusion

$$\frac{\partial c}{\partial \tau} + u \frac{\partial c}{\partial x} + v \frac{\partial c}{\partial y} + Q(c) = D \left(\frac{\partial^2 c}{\partial x^2} + \frac{\partial^2 c}{\partial y^2} \right) \quad (1.1)$$

and by the continuity equation

$$\frac{\partial u}{\partial x} + \frac{\partial v}{\partial y} = 0. \quad (1.2)$$

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Generally, the velocity field (u, v) is assumed to be nonuniform and known within the framework of the present analysis. This field is to be found as a solution of an appropriate hydrodynamic problem. In (1.1), c is the local concentration, D is the molecular diffusivity, $Q(c)$ is the intensity of the source of mass related, in particular, to chemical transformations, x and y are the spatial Cartesian coordinates, and τ is the time. The impurity substance is dynamically passive, i.e., its spreading does not affect the liquid flow in the channel. The velocity field may be arbitrary, but the no-slip condition should be fulfilled at the channel walls:

$$u \Big|_{y=0;h} = v \Big|_{y=0;h} = 0. \quad (1.3)$$

Below, we will show that some integral characteristics of the velocity field will only be necessary.

The model is supplemented with the initial condition

$$c \Big|_{\tau=0} = c_0(x, y) \quad (1.4)$$

and the boundary condition

$$\frac{\partial c}{\partial y} \Big|_{y=0;h} = 0. \quad (1.5)$$

The conditions over the variable x are of no use in deriving the simplified system of equations; therefore, for the time being, their particular form is of no interest. Relations (1.5) express the absence of any flux of the substance at the channel walls.

Note some difficulties that arise in the numerical analysis of problem (1.1)–(1.5) (with allowance for the boundary conditions over the variable x) in the case of flows with closed (or almost closed) streamlines. An important property of such problems is variation of the characteristic time and spatial scales of variables during the process: boundary layers appear and disappear, the substance concentration levels out along certain directions, etc. These phenomena cause substantial difficulties in predicting the process in the entire space and over long time intervals. In fact, different numerical algorithms are to be used to solve one and the same problem in different space–time regions. The necessity of passing to a new scheme (in the simplest case, to a different step in finite-difference methods) is hard to notice since the scales of variables vary by orders of magnitude in extreme situations.

The alteration of the mass-transfer mechanism in flows with closed streamlines in a bounded space is also often observed in other problems similar to those considered in the present study. Heat and mass exchange between a liquid drop and the surrounding flow has been extensively examined (see, e.g., [8, 9]). In [8, 9], various mechanisms of mass-transfer alteration and difficulties that arise in the description of the whole process with one model are discussed. Note also that the methods of problem solution have been many times discussed (see, e.g., [10]) in connection with discrepancies between results obtained by different authors. An analysis of [8, 9] and other works shows that the models discussed in [10], and some other models, adequately describe the process only in certain space–time regions.

Within the framework of the Taylor theory, problem (1.1)–(1.5) can be reduced to the form [11]

$$\frac{\partial C}{\partial \tau} + U \frac{\partial C}{\partial x} + Q(C) = \frac{\partial}{\partial x} \left[(D + D_*(x)) \frac{\partial C}{\partial x} \right], \quad (1.6)$$

where U is the mean flow velocity, C is the concentration of the substance averaged over the channel cross section, and $D_*(x)$ is the convective component of the dispersion coefficient (the total dispersion coefficient is $D + D_*$). The mean (averaged over the channel cross section) value of a function $F(x, y, \tau)$ is given by the formula

$$\langle F(x, \tau) \rangle = \frac{1}{h} \int_0^h F(x, y, \tau) dy. \quad (1.7)$$

The value of D_* in (1.6) can be found from the expression

$$D_*(x) = \langle \psi^2 \rangle / D, \quad (1.8)$$

where $\psi(x, y)$ is the stream function in a coordinate system that moves with a mean velocity U determined from the equations

$$u = U + \frac{\partial \psi}{\partial y}, \quad v = -\frac{\partial \psi}{\partial x}. \quad (1.9)$$

For the sake of convenience, the x direction is chosen to coincide with the direction of the mean velocity vector, i.e., in what follows, $U \geq 0$. Note that the mean velocity U does not depend on the coordinate x . Indeed, relations (1.2), (1.3), and (1.7) yield

$$\frac{\partial U}{\partial x} = \left\langle \frac{\partial u}{\partial x} \right\rangle = - \left\langle \frac{\partial v}{\partial y} \right\rangle = \frac{v}{h} \Big|_{y=h}^{y=0} = 0,$$

i.e., $U = \text{const}(x)$.

Clearly, for an analysis of general problems, Eq. (1.6) is much simpler than system (1.1), (1.2); yet, the use of (1.6) is limited to the case of weak sources of the substance $Q(C)$ and sufficiently long characteristic times of the process. In view of this, we generalize Eq. (1.6) to construct a system of equations defining models similar to relaxation (or wave) models of longitudinal mixing.

In deriving hyperbolic-type equations for substance spreading, various iteration methods [4, 12, 13], expansion of the solution in terms of certain functions [5], and a generalized Galerkin method [6, 7] were used. The experience shows that an acceptable approximation of known exact solutions can be obtained using an approximation containing a system of two equations, which corresponds to two basic function in the Galerkin method. In particular, Dil'man and Kronberg [5] found with some examples, by means of a comparison with exact solutions, that allowance for the third term in the Galerkin-type expansions only insignificantly improves the calculation accuracy, whereas the search for the solution becomes more difficult. In view of the aforesaid, we seek the solution of problem (1.1)–(1.5) in the form of the sum of two functions (truncated series) of the Galerkin method:

$$c(x, y, \tau) = C(x, \tau) + R(y)j(x, \tau). \quad (1.10)$$

Here, the first Galerkin expansion function is unity, and the second Galerkin expansion function is the function $R(y)$ that satisfies the following requirements:

$$R'(0) = R'(h) = 0, \quad \langle R \rangle = 0, \quad \langle R^2 \rangle = 1. \quad (1.11)$$

In (1.11), the first two relations satisfy the boundary conditions (1.5), and the third relation satisfies the condition of orthogonality of the functions 1 and $R(y)$ [this condition defines the function $C(x, \tau)$ as the concentration of the target substance averaged over the channel cross section], and the last relation is the normalization condition.

We substitute (1.10) into (1.1); then, according to the Galerkin procedure, we demand that the expression (residual) obtained be orthogonal to a chosen system of functions [the functions 1 and $R(y)$ in the case under consideration]. Here, the orthogonality implies that the product of the two functions integrated over y in the limits $(0, h)$ be zero. After some rearrangements, using (1.2), (1.3), and (1.11), we obtain the system

$$\frac{\partial C}{\partial \tau} + U \frac{\partial C}{\partial x} + \frac{\partial}{\partial x} [K(x)j] + Q(C) = D \frac{\partial^2 C}{\partial x^2}, \quad (1.12)$$

$$\frac{\partial j}{\partial \tau} + V(x) \frac{\partial j}{\partial x} + K(x) \frac{\partial C}{\partial x} + \left[\frac{V'(x)}{2} + Q'(C) + \frac{1}{\vartheta} \right] j = D \frac{\partial^2 j}{\partial x^2}, \quad (1.13)$$

where the parameters K , V , and ϑ are defined by the expressions

$$K(x) = \langle uR \rangle, \quad V(x) = \langle uR^2 \rangle, \quad \vartheta^{-1} = D \langle (R')^2 \rangle. \quad (1.14)$$

In deriving (1.12) and (1.13), the source function $Q(c)$ in (1.1) was approximated by the truncated Taylor series $Q(c) \cong Q(C) + Q'(C)Rj$. The choice of the point C for the expansion of $Q(c)$ in its vicinity is motivated by the fact that this quantity defines the first (principal) term in representation (1.10); for this reason, the second term Rj in (1.10) is a correction one. Note that such an approximation becomes an exact equality if the function $Q(c)$ is linear (first-order reaction).

If the function $Q(C)$ is a nonlinear, abruptly changing function [the derivative $Q'(C)$ is large], there may become necessary a closer approximation to the expressions

$$\langle Q(C + jR) \rangle, \quad \langle RQ(C + jR) \rangle, \quad (1.15)$$

which must enter (1.12) and (1.13) instead of the terms $Q(C)$ and $jQ'(C)$, respectively. In some cases, for instance, for a second-order reaction, for which $Q(c) = k_2 c^2$ ($k_2 = \text{const}$), the averaging in (1.15) can be performed. We have

$$k_2(C^2 + j^2), \quad k_2(2Cj + j^2 \langle R^3 \rangle).$$

Otherwise, the integrals in (1.15), implied by the averaging procedure (1.7), may have to be calculated.

2. Relation with the Taylor Diffusion Model. We nondimensionalize system (1.12), (1.13):

$$\frac{\partial C}{\partial t} + \frac{\partial C}{\partial z} + \frac{1}{\varepsilon_K \text{Pe}_*} \frac{\partial}{\partial z} [k(z)j] + \Phi(C) = \frac{1}{\text{Pe}} \frac{\partial^2 C}{\partial z^2}; \quad (2.1)$$

$$\varepsilon_U \left(\frac{\partial j}{\partial t} + w(z) \frac{\partial j}{\partial z} \right) + \varepsilon_K k(z) \frac{\partial C}{\partial z} + \left[1 + \frac{\varepsilon_U w'(z)}{2} + \varepsilon_Q \Phi'(C) \right] j = \frac{\varepsilon_U}{\text{Pe}} \frac{\partial^2 j}{\partial z^2}. \quad (2.2)$$

Here $w = V/U$ [we assume that $w = O(1)$, i.e., the quantity U (we set $U \neq 0$) serves as the scale of the variable $V(x)$], $\varepsilon_U = \vartheta U/L$ is the parameter indicative of the relative effects of the relaxation time ϑ and the transfer time $T_U = L/U$ on the process, $\varepsilon_Q = \vartheta/T_Q$ is the ratio between the characteristic relaxation time (ϑ) and the characteristic time of chemical transformation (T_Q), L is the length of the channel, $t = \tau/T_U$, and $z = x/L$. The quantity T_Q is reciprocal to the scale of the reaction-rate derivative dQ/dc (Q and c are dimensional parameters). We denote the scale of the function $K(x)$ as K_* [i.e., $k(z)$ is the dimensionless value of $K(x)$]; then, for the parameter ε_K , we have $\varepsilon_K = \vartheta K_*/L$. Next, $\Phi(C) = Q(C)L/U$ is the dimensionless rate of the chemical reaction [here, the scale of dQ/dc defines T_Q and not the quantity T_U that enters the definition of the function $\Phi(C)$] and $\text{Pe}_* = UL/(\vartheta K_*^2) = UL/D_*$ since, as is shown below, the quantity ϑK_*^2 is the scale of the Taylor dispersion coefficient. Here, the dispersion coefficient can be found from the relation $D_* = K^2(x)\vartheta$ ($D_* > 0$). Thus, Pe_* is the Peclet number for the convective component of the dispersion coefficient. The Peclet number based on the ordinary (molecular) diffusivity D can be found as $\text{Pe} = UL/D$.

Several dimensionless parameters (ε_U , ε_Q , ε_K , Pe_* , and Pe) governing the process as described by system (2.1), (2.2) make it possible to consider several simplified (extreme) situations with some limiting relations held between these parameters and unity. Below, we consider some typical cases, often met in practice, in which $\varepsilon_U \ll 1$, $\text{Pe} \gg 1$, and $\text{Pe} \gg \text{Pe}_*$, under the assumption that other parameters, if retained in the equations, are of the order of unity.

The passage to the diffusion model occurs if the parameters ε_U and ε_Q are negligibly small, i.e., the shortest time scale in the system is the relaxation time ϑ , and of interest are processes with the characteristic time T_U . With $\varepsilon_U \ll 1$ and $\varepsilon_Q \ll 1$, Eq. (2.2) yields $j = -[\varepsilon_K k(z)]\partial C/\partial z$, a relation being a kind of dimensionless Fick law; substitution of this relation into (2.1) yields the dimensionless equation of the diffusion model

$$\text{Pe}_* \left(\frac{\partial C}{\partial t} + \frac{\partial C}{\partial z} + \Phi(C) \right) = \frac{\partial}{\partial z} \left[\left(D^*(z) + \frac{\text{Pe}_*}{\text{Pe}} \right) \frac{\partial C}{\partial z} \right], \quad (2.3)$$

where $D^* = k^2(z)$ is the dimensionless Taylor diffusivity.

For the Peclet number Pe_* to be of the order of unity, the limiting inequality $U \ll K_*$ must be fulfilled at $T_U \gg \vartheta$, i.e., the longitudinal velocity averaged by the first expression in (1.14) must be much higher than the mean velocity. Rather intense mixing is observed in the system since, by virtue of the third relation in (1.11), the time-independent velocity component (in particular, U) does not affect the result of averaging in determining $K(x)$, i.e., here, in fact, the fluctuating velocity is averaged.

It should be noted that, for the inequalities $\text{Pe} \gg 1$ and $\text{Pe} \gg \text{Pe}_*$, which normally hold, the terms in the right side of (2.1) and (2.2) can usually be omitted. This also applies to the term in (2.3) that contains the factor Pe_*/Pe . Yet, the indicated terms play an important role at the interfaces between the circulation zones, where the normal component of the flow velocity vanishes and the parameter K and the effective diffusivity D_* also vanish. The convective motion rather rapidly levels out the concentration of the substance within each closed circulation zone; nonetheless, because of the equality $D_* = 0$, the mass transfer between the zones is conditioned by ordinary diffusion, i.e., proceeds much more slowly. The convective flow in the contact zones between the cells just supplies the substance to the interface but does not participate in the transfer through the interface, since the transport velocity is parallel to the interfacial surface.

At the initial stage, rapid processes with a characteristic scale ϑ are possible. In this case, Eq. (2.1) supplements the equation similar to the Maxwell relaxation law with a spatially dependent coefficient, yielded by (2.2) with $\varepsilon_U \rightarrow 0$ and $\varepsilon_Q \rightarrow 0$

$$\varepsilon_U \frac{\partial j}{\partial t} + \varepsilon_K k(z) \frac{\partial C}{\partial z} + j = 0, \quad (2.4)$$

where the time-dependent term cannot be ignored over short times.

Note that the variable j is related to the flux of the substance J as $J = K(x)j$. We use the variables j and K separately since these variables are introduced in the theory separately. In addition, the passage to the variable J for $K(x) \neq \text{const}$ in system (2.1), (2.2) somewhat complicates the latter. The passage to the flux J in (1.12) and (2.4) makes it possible to write the system of relaxation-type equations in dimensional form:

$$\frac{\partial C}{\partial \tau} + U \frac{\partial C}{\partial x} + \frac{\partial J}{\partial x} + Q(C) = D \frac{\partial^2 C}{\partial x^2}, \quad \vartheta \frac{\partial J}{\partial \tau} + D_*(x) \frac{\partial C}{\partial x} + J = 0, \quad D_*(x) = K^2(x)\vartheta.$$

Normally, the relaxation time ϑ is shorter than the characteristic time $T_U = L/U$, and the inequality $\vartheta \ll T_Q$ may often be violated. In the case of a first-order reaction [$Q(c) = k_1c$], we have $T_Q = 1/k_1$ and, for the diffusion model to be applicable, the limiting inequality $\vartheta k_1 \ll 1$ must be fulfilled. The worsened accuracy in calculations by the diffusion model compared to that in calculations by the master equation of convective diffusion, when the relation $\vartheta k_1 = O(1)$ or $\vartheta k_1 \gg 1$ holds, was established in [5, 6]. Under the same conditions, the relaxation model also yields satisfactory results if $\vartheta k_1 \gg 1$.

Consider some examples in which one of the inequalities $\vartheta \ll T_U$ or $\vartheta \ll T_Q$ is violated. The case of $\vartheta \ll T_Q$ and $\varepsilon_U = O(1)$ is of no interest because, here, we have only an insignificant simplification of the proposed model [namely, the term $\varepsilon_Q \Phi'(C)$ in Eq. (2.2) can be omitted]. More interesting is the case in which the inequality $\vartheta \ll T_U$ holds and the relation $\vartheta \ll T_Q$ is violated. Then, Eq. (2.2) yields the Fick law in which the diffusion (dispersion) coefficient depends on the concentration of the target substance: $j = -\varepsilon_K k(z)[1 + \varepsilon_Q Q'(C)]^{-1} \partial C / \partial z$. We write the dispersion equation following from Eq. (1.12) in dimensional form

$$\frac{\partial C}{\partial \tau} + U \frac{\partial C}{\partial x} + Q(C) = \frac{\partial}{\partial x} \left(D_0(C, x) \frac{\partial C}{\partial x} \right), \quad (2.5)$$

where $D_0(C, x) = D_*(x)/[1 + \vartheta Q'(C)] + D$ is the modified dispersion coefficient.

Yet, it should be noted that the quantity $D_0(C, x)$ in (2.5) can be regarded as a coefficient analogous to the diffusion coefficient only if $D_0(C, x) > 0$ in the region under consideration, which implies that the inequality $1 + \vartheta Q'(C) > 0$ or $1 + \vartheta Q'(C) < -D_*(x)/D$ must be fulfilled, since both the Taylor coefficient D_* and the diffusivity D are always positive. The first inequality can be violated if the kinetic function $Q(C)$ sharply decreases somewhere [$Q'(C) < -1/\vartheta$]. The second inequality is violated if $D_* \gg D$, which is normally the case in practice. For the case with an autocatalytic source of the substance considered in [14, 15], we have $Q(C) = bC/(g + C)^2$ ($b > 0$, $g > 0$), and the modified dispersion coefficient $D_0(C, x)$ is always positive in the region $C > 0$, provided that the condition $b\vartheta < 27g^2$ is fulfilled. Otherwise, with a sufficiently high value of $D_*(x)/D$ in the region of positive concentrations, the coefficient $D_0(C, x)$ is negative over a certain interval of concentrations. In this case, the passage from the relaxation to the diffusion model seems to be unreasonable. Note that the dependence of the dispersion coefficient on the parameters of the mass source for a first-order chemical reaction was mentioned in [12].

3. The Choice of the Function R in the Galerkin Method. The system of functions of the Galerkin method should be matched to additional conditions, solution properties, etc. A proper choice of basic functions of the method can provide a better approximation to the exact solution and allows one to consider a smaller number of equations. These functions should be chosen as simple as possible, so that the integrals could be integrated analytically. In the present work, the function R was chosen in the form of a polynomial satisfying the largest possible number of conditions matching a particular problem under consideration.

In addition to the fulfillment of conditions (1.11), it is desirable that the dispersion coefficients of the diffusion model (1.8) in their limiting form be coincident with the dispersion coefficients of the relaxation model:

$$\langle \psi^2 \rangle = DK^2\vartheta = \langle uR \rangle^2 / \langle (R')^2 \rangle.$$

Nonetheless, by virtue of the Cauchy–Bunyakovskii inequality and by the definition (1.9) of the stream function, we have

$$\langle uR \rangle^2 = \left(\frac{\psi R}{h} \Big|_0^h - \langle \psi R' \rangle \right)^2 = \langle \psi R' \rangle^2 \leq \langle \psi^2 \rangle \langle (R')^2 \rangle,$$

i.e., the dispersion coefficient in the diffusion model, given by (1.8), is greater than the dispersion coefficient in the present model. Equality between these coefficients is possible if the functions ψ and R' vary in proportion to each other. Yet, the stream function generally depends on two coordinates, whereas, for convenience, the function $R(R')$ is chosen to depend only on y . In a particular case of the Poiseuille flow in a plane channel, the stream function depends only on y , and we can make the dispersion coefficients be coincident, at least, in this particular problem.

Here, the stream function can be expressed in terms of y as the polynomial $\psi = Uh(3\eta^2 - 2\eta^3 - \eta)$, where $\eta = y/h$. We set the latter expression, taken with an indefinite multiplier, equal to $R'(y)$, perform integration, and use two integral conditions (1.11); then, we find the constant of integration and the indicated multiplier. In this way, we obtain the following expression for the function R :

$$R(y) = \sqrt{7/3} (1 + 60\eta^3 - 30\eta^4 - 30\eta^2), \quad \eta = y/h. \quad (3.1)$$

Formula (3.1) allows one to find the general expression for the relaxation time ϑ [see (1.14)]:

$$\vartheta = h^2/(40D).$$

4. Hyperbolic System of Transport Equations. We assume that $Pe \gg 1$, and the coefficient K is not constant but is separated from zero by a certain interval. Then, the right sides of the equations in the dimensional system (1.12), (1.13) and in the dimensionless system (2.1), (2.2) can be neglected. Following [16], we establish the main properties of the system thus obtained. To this end, we write the system in the matrix form, isolating terms with derivatives, and find the eigenvalues of the resultant matrix [16]. We write system (1.12), (1.13) with a zero right side as

$$\frac{\partial S}{\partial \tau} + A(x) \frac{\partial S}{\partial x} + BS = f, \quad S = \begin{pmatrix} C \\ j \end{pmatrix}, \quad A(x) = \begin{pmatrix} U & K(x) \\ K(x) & V(x) \end{pmatrix}, \quad (4.1)$$

where the components of the matrices B and f can be determined from (1.12) and (1.13). These matrices are of no help in establishing the main properties of the system; hence, they are not presented here. The eigenvalues λ of the matrix $A(x)$ are determined by the equation

$$|A(x) - \lambda(x)E| = 0 \quad (4.2)$$

(E is a unit matrix). Expanding determinant (4.2), we obtain a quadratic equation with respect to λ :

$$\lambda^2 - (U + V)\lambda + \Delta = 0, \quad \Delta = UV - K^2. \quad (4.3)$$

The discriminant of (4.3) is $(U - V)^2 + 4K^2$. This discriminant is always positive and, hence, the roots of (4.3) are real-valued and not multiple, i.e., system (4.1) is of hyperbolic type. The key role in setting additional conditions for this system belongs to the parameter $\Delta = UV - K^2$ equal to the determinant of the matrix $A(x)$.

Let the mass-transfer process proceeds in the region $x \in (0, L)$. For definiteness, the x direction is chosen to coincide with the direction of the mean-velocity vector, i.e., $U > 0$. It is easy to see that the largest root of (4.3), $\lambda_+ = 0.5\{U + V + [(U - V)^2 + 4K^2]^{1/2}\}$, is always positive, whereas the sign of the second root, $\lambda_- = 0.5\{U + V - [(U - V)^2 + 4K^2]^{1/2}\}$, coincides with that of Δ . Three cases are possible: $\Delta > 0$, $\Delta < 0$, and $\Delta = 0$ at some point x .

Case 1: $\Delta > 0$ at all points $x \in (0, L)$. In this case, the slope of both characteristics (the sign of wave velocities) $dx_{\pm}/d\tau = \lambda_{\pm}(x)$ is positive; two boundary conditions for system (4.1) are, therefore, to be posed at the left boundary of the region ($x = 0$) and no condition at $x = L$. This variant of the system with constant coefficients, which refers to substance spreading in the Poiseuille flow in a round pipe, was examined by Dil'man and Kronberg [5, 6].

We show that $\Delta > 0$ in the case of a unidirectional (directed along the x axis) liquid flow with $u(x, y) \geq 0$. In the case of a turbulent liquid flow, the function $u(x, y)$ is understood as an averaged (fluctuation-free) value of the flow velocity. For this to become evident, note that the inequality $\Delta > 0$, i.e., $UV > K^2$, for $u \geq 0$ is equivalent to the integral Cauchy–Bunyakovskii inequality. Indeed,

$$K^2 = \langle uR \rangle^2 = \langle \sqrt{u} R \sqrt{u} \rangle^2 \leq \langle u \rangle \langle uR^2 \rangle = UV,$$

since the square root of u is real.

In calculating the coefficients of the hyperbolic model, it was common practice [5, 6] to use the known velocity profiles in piped flows in laminar and turbulent flow modes. In this case, $u \geq 0$ (for the turbulent motion, this is the averaged velocity without turbulent fluctuations), i.e., in view of the aforesaid, $\Delta > 0$. This case was examined in sufficient detail.

For all values of Δ , two families of characteristics emerge from the line $\tau = 0$ into the region $\tau > 0$, $x \in (0, L)$ under consideration. That is why two (initial) conditions should be posed at this line [16]. These conditions are obtained by the averaging procedure (1.7) applied to the initial distribution of the concentration $c_0(x, y)$ (1.4),

related to the Galerkin expansion (1.10). This can be easily verified since the standard procedure of the Galerkin method (requirement of orthogonality of the residual resulting from the substitution of the Galerkin expansion into some equality to the system of chosen functions) is equivalent to averaging of this equality sequentially multiplied by each function of the Galerkin system. We have

$$C\Big|_{\tau=0} = \langle c_0 \rangle, \quad j\Big|_{\tau=0} = \langle Rc_0 \rangle. \quad (4.4)$$

The initial concentration is often assumed to be independent of the crossflow coordinate y . In the first relation of (4.4), the averaging sign can be omitted, and the second relation yields, in view of (1.11), the equality $j(x, 0) = 0$. The same assumptions are also normally adopted for the concentration of the substance at the inlet to the system, $c_+(0, y, \tau) = \text{const}(y) = c_+(\tau)$. We are going now to obtain the boundary conditions for system (4.1). To this end, we apply the averaging procedure in the Galerkin method to the balance (conservation law) of the substance at the inlet to the system:

$$u(0, y)c_+(\tau) = u(0, y)[C(0, \tau) + R(y)j(0, \tau)]. \quad (4.5)$$

The direct averaging of (4.5) and subsequent averaging with the weight $R(y)$ yield the system of linear equations for $C(0, \tau)$ and $j(0, \tau)$

$$UC(0, \tau) + K(0)j(0, \tau) = Uc_+(\tau), \quad K(0)C(0, \tau) + V(0)j(0, \tau) = K(0)c_+(\tau) \quad (4.6)$$

with the determinant $\Delta(0) > 0$. We found from here that this system has a single solution of the form

$$C\Big|_{x=0} = c_+(\tau), \quad j\Big|_{x=0} = 0. \quad (4.7)$$

Case 2: $\Delta(0) = 0$. In this case, only one system of characteristics λ_+ emerges from the line $x = 0$ into the region $\tau > 0$, $x \in (0, L)$, and no characteristics emerge from the line $x = L$. Here, relation (4.5) is to be used to perform only one averaging, and the preference should be given to the averaging with the first function of the Galerkin method, i.e., with the unit function. Thus, we obtain the first equality in (4.6):

$$(CU + jK)\Big|_{x=0} = Uc_+(\tau). \quad (4.8)$$

Case 3: $\Delta(0) < 0$. In this case, a system of characteristics λ_+ emerges from the line $x = 0$ into the region $\tau > 0$, $x \in (0, L)$. As in the second case, the boundary condition (4.8) is fulfilled. At the outlet from the system (at $x \geq L$), similarly to the situation at the inlet to the system, we assume that the concentration c_- does not depend on y . We assume that the function $c_-(\tau)$ is unknown. Constructing a system analogous to (4.6) in the cross-section $x = L$ and obtaining the single (for $\Delta < 0$) solution of the type (4.7), for the boundary conditions with known functions to be constructed, we chose the second condition

$$j\Big|_{x=L} = 0 \quad (4.9)$$

in addition to (4.8) for the hyperbolic system with $\Delta < 0$. Note that this variant ($\Delta < 0$) is always the case for stagnant caverns, for which $U = 0$ and $\Delta = -K^2 < 0$.

The proposed boundary conditions (4.7) for $\Delta > 0$, (4.8) for $\Delta = 0$, and (4.8) and (4.9) for $\Delta < 0$ do not exhaust all possible variants of boundary conditions; they are considered here because they are analogous to the Dankwerts conditions

$$D_* \frac{\partial C}{\partial x}\Big|_{x=0} = U[C - c_+(\tau)], \quad \frac{\partial C}{\partial x}\Big|_{x=L} = 0 \quad (4.10)$$

widely used in the diffusion model. Recall that the diffusion model stems from the hyperbolic one in the limiting situation ($\varepsilon_U \ll 1$, $\varepsilon_Q \ll 1$) where the flux is related to the gradient of mean concentration by the Fick law $j = -\vartheta K(x) \partial C / \partial x$. In the limiting transition, case 3 ($\Delta < 0$) of the hyperbolic model is realized, and formulas (4.8), (4.9) and the equality $D_* = K^2(x)\vartheta$ yield (4.10).

The diffusion model with the Dankwerts conditions (4.10) has gained widespread application in analyzing many natural and technological processes. As was shown above, case 3 ($\Delta < 0$) of the hyperbolic model proved to be most close to this model, since it also represents a boundary-value problem. This circumstance seems to hamper the practical application of the hyperbolic model that had initially emerged in the case of $\Delta > 0$ [5, 6], which refers

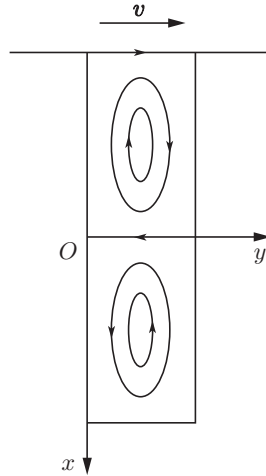


Fig. 1. Flow over a cavity.

to the Cauchy problem with respect to the variable x [conditions (4.7)], despite the fact that the calculations by the hyperbolic model proved to better agree with the exact solutions.

5. Calculation of the Coefficient of Mass Transfer between Cavities. As an example of using system (1.12), (1.13), let us determine the coefficient of mass transfer between cavities; in this way, we generalize the results of [17] obtained by the diffusion model. Here, we rely upon the relations between parameters normally met in practice.

In view of (1.8), the diffusion model (1.6) contains the following inequality for the total dispersion coefficient:

$$D_* + D \geq 2\langle\psi^2\rangle^{1/2},$$

i.e., the dispersion coefficient is restricted from below. Yet, the convective component of D_* is considerably higher than the molecular component D almost throughout the whole volume of the system, and only in those regions where $D_* = 0$ is the role of the coefficient D substantial. The latter necessitates consideration of the problem in the boundary-layer approximation [17]. A similar situation arises in the analysis of the problem based on Eqs. (1.12) and (1.13). Of importance are regions where the function $K(x)$ vanishes (recall that $D_* = K^2\vartheta$). The problem will be considered for non-reacting flows in stagnant cavities ($U = 0$). Such a situation is realized, for instance, when a cavity contains a flow whose flow pattern is given by the Lavrent'ev diagram [18], which implies that several circulation zones can be observed (Fig. 1). The interface between the zones is assumed to be a straight segment at $x = 0$ (normally, this boundary is somewhat bent). Everywhere in this line, we have $u = 0$. In the boundary-layer approximation ($K_*^2\vartheta \gg D$), in a vicinity of the line $x = 0$, we can restrict the consideration to the first terms of the Taylor series for the functions $K(x)$ and $V(x)$. We have

$$K(x) = \varkappa x, \quad V(x) = \mu x, \quad \varkappa = \left\langle \frac{\partial u}{\partial x} R \right\rangle \Big|_{x=0}, \quad \mu = \left\langle \frac{\partial u}{\partial x} R^2 \right\rangle \Big|_{x=0}. \quad (5.1)$$

Next, we assume that $\varkappa \neq 0$. This parameter can be zero if the derivative $\partial u/\partial x$ [or $\partial v/\partial y$ by virtue of continuity equation (1.2)] is orthogonal at $x = 0$ to the second function $R(y)$ of the orthogonal Galerkin system. If we restrict the consideration to the analysis of the binomial expansion (1.10), then it seems not to be logical to relate the derivative $\partial v/\partial y$ to higher Galerkin-expansion functions. That is why the case $\partial v/\partial y = \text{const}$ at $x = 0$ seems to be realistic. From the no-slip condition at $y = 0$ and $y = h$, it follows, after integration over y , that $v = 0$. The latter means that the interfacial line $x = 0$ is equivalent to a rigid boundary since, there, $u = v = 0$. The latter is the case at the cavity bottom. A quadratic approximation of the function $K(x)$ is necessary in analyzing mass transfer at a rigid surface (with $\varkappa = 0$), as well as at the surface moving with a velocity $v = \text{const}$ along the y axis. To calculate the coefficients \varkappa and μ from the entire velocity field by formula (5.1), one has to know only the value of v at the interface between the cells. Provided that a power approximation of v at $x = 0$ is used, it suffices only to determine terms up to the order of y^7 inclusive, since both the function $R(y)$ and the function $v(0, y)$ can be

expanded into a system of orthogonal functions [Legendre polynomials with the passage to the interval $(-1, +1)$]; here, the polynomials of higher-than-seventh orders do not affect the calculation of μ , and the polynomials of higher-than-third orders, the calculation of α .

Thus, the system of mass-transfer equations under the above-made assumptions in the vicinity of the interfacial line between the circulation zones is

$$\frac{\partial C}{\partial \tau} + \frac{\partial}{\partial x} (\alpha x j) = D \frac{\partial^2 C}{\partial x^2}; \quad (5.2)$$

$$\frac{\partial j}{\partial \tau} + \mu x \frac{\partial j}{\partial x} + \alpha x \frac{\partial C}{\partial x} + \left(\frac{\mu}{2} + \frac{1}{\vartheta} \right) j = D \frac{\partial^2 j}{\partial x^2}. \quad (5.3)$$

Since system (5.2), (5.3) contains solutions of the boundary-layer type, the boundary conditions for this system are

$$C \Big|_{x \rightarrow \pm \infty} \rightarrow C_{\pm}, \quad j \Big|_{x \rightarrow \pm \infty} < \infty, \quad (5.4)$$

where C_{\pm} is the concentration of the substance in neighboring cavities far from the interface. Similar problems were previously discussed in [11, 17]; from these studies, we can conclude that mass transfer between the cavities can be predicted over the time interval under consideration by using the quasi-stationary approximation; i.e., to calculate the coefficient of transfer between the circulation regions, one should use the stationary solution of problem (5.2)–(5.4). Here, the values of C_{\pm} correspond, with acceptable accuracy, to the concentrations of the target substance averaged over the circulation regions. Since the transport velocity at the interface between the cells is parallel to the interface, the mass transfer between the cells is controlled by molecular diffusion. For the coefficient ζ of exchange of the substance between the cells through the boundary $x = 0$, following [17], we derive the formula

$$\zeta = \frac{D}{l \delta C} \frac{dC}{dx} \Big|_{x=0}, \quad \delta C = C_+ - C_-, \quad (5.5)$$

where l is the length of the cavity.

We write the stationary equations (5.2), (5.3) in dimensionless variables:

$$q = \frac{j}{\delta C}, \quad H = \frac{C}{\delta C}, \quad \frac{\xi}{x} = \sqrt{\frac{\alpha}{D \sin 2\varphi}}, \quad 2\nu + 1 = \frac{\sin 2\varphi}{\vartheta \alpha}. \quad (5.6)$$

The angle φ is defined by two equations

$$\sin 2\varphi = \frac{2\alpha}{\sqrt{\mu^2 + 4\alpha^2}}, \quad \tan 2\varphi = \frac{2\alpha}{\mu}, \quad (5.7)$$

where the square root is to be understood arithmetically. Generally, if the sign of α is opposite to that of μ , we can assume that $\varphi \in (-\pi/2, \pi/2)$. Thus, φ is a single-valued function of α and μ . From (5.2), (5.3), and (5.6), we obtain

$$\sin 2\varphi \frac{d}{d\xi} (\xi q) = \frac{d^2 H}{d\xi^2}; \quad (5.8)$$

$$\xi \sin 2\varphi \frac{dH}{d\xi} + 2\xi \cos 2\varphi \frac{dq}{d\xi} + [2\nu + 1 + \cos 2\varphi] q = \frac{d^2 q}{d\xi^2}. \quad (5.9)$$

The first integral of (5.8) is

$$\xi q \sin 2\varphi + A = \frac{dH}{d\xi}, \quad (5.10)$$

where A is the constant of integration, related to the mass-transfer coefficient ζ [see (5.5)]; the quantity A is, in a sense, the dimensionless value of ζ [see (5.12)]. We make the change $q \sin 2\varphi = -AZ$; then, from (5.9), we obtain the following equation for the new sought function Z :

$$\frac{d^2 Z}{d\xi^2} = 2\xi \cos 2\varphi \frac{dZ}{d\xi} + [2\nu + 1 + \cos 2\varphi + \xi^2 \sin^2 2\varphi] Z - \xi \sin^2 2\varphi. \quad (5.11)$$

We integrate (5.10) within infinite limits; then, using (5.10) at $\xi = 0$, we obtain the following expression for the mass-transfer coefficient ζ in (5.5):

$$\frac{1}{A} = \frac{1}{l\zeta} \sqrt{\frac{aeD}{\sin 2\varphi}} = \int_{-\infty}^{\infty} [1 - \xi Z(\xi)] d\xi. \quad (5.12)$$

Formula (5.12) shows that, in calculation of ζ , only the odd component of the function $Z(\xi)$ in its expansion $Z(\xi) = 0.5[Z(\xi) + Z(-\xi)] + 0.5[Z(\xi) - Z(-\xi)]$ is important. Therefore, we first find the odd solution of (5.11).

We make the change of the sought function $Z(\xi) = Y(\xi) \exp[(\xi^2 \cos 2\varphi)/2]$. For the new function $Y(\xi)$, we obtain

$$\frac{d^2 Y}{d\xi^2} - (2\nu + 1 + \xi^2)Y + \xi \sin^2 2\varphi \exp\left(-\frac{\xi^2 \cos 2\varphi}{2}\right) = 0. \quad (5.13)$$

This equation is related to Hermit functions. Its odd solution, bounded at infinity, has the form

$$Y(\xi) = Y_1(\xi) \int_0^\xi Y_2(x)\sigma(x) dx + Y_2(\xi) \int_\xi^\infty Y_1(x)\sigma(x) dx, \quad (5.14)$$

$$\sigma(x) = x \sin^2 2\varphi \exp\left(-\frac{x^2 \cos 2\varphi}{2}\right),$$

where

$$Y_1(x) = \exp\left(-\frac{x^2}{2}\right) H_{-1-\nu}(x), \quad (5.15)$$

$$Y_2(x) = Y_1(x) \int_0^x \frac{d\xi}{Y_1^2(\xi)} = \frac{\Gamma(1+\nu)}{2^{-\nu}\sqrt{\pi}} \exp\left(-\frac{x^2}{2}\right) [H_{-1-\nu}(-x) - H_{-1-\nu}(x)].$$

Here $\Gamma(x)$ is the Euler gamma-function and $H_\nu(x)$ is the Hermit function of the corresponding index [19]. Formulas (5.14) and (5.15) allow us to establish the properties of the function Y required in the limiting cases for subsequent calculations.

Let us obtain the expansion of Y in Hermit polynomials. The functions $S_k = \exp(-\xi^2/2)H_k(\xi)$, where $k = 0, 1, 2, \dots$, are known to satisfy the equations [19]

$$\frac{d^2 S_k}{d\xi^2} + (2k + 1 - \xi^2)S_k = 0. \quad (5.16)$$

We multiply Eq. (5.16) by Y and Eq. (5.13) by S_k and subtract the results. Next, we integrate the resultant expression with respect to ξ between infinite limits, taking into account the asymptotic behavior of the functions Y and S_k as $\xi \rightarrow \pm\infty$. As a result, we obtain the relation

$$2(\nu + k + 1) \int_{-\infty}^{\infty} Y S_k d\xi = \sin^2 2\varphi \int_{-\infty}^{\infty} \xi S_k d\xi \exp\left(-\frac{\xi^2 \cos 2\varphi}{2}\right) \quad (5.17)$$

that relates the coefficients of expansion of the functions $Y(\xi) \exp(\xi^2/2)$ and $\xi \exp[\xi^2/2 - (\xi^2 \cos 2\varphi)/2] = \xi \exp[\xi^2 \sin^2 \varphi]$ into the series in Hermit polynomials with the weight $\exp(-\xi^2)$. In [19], the following expansion is reported, written in variables convenient for the present consideration:

$$\exp(x^2 \sin^2 \varphi) = \frac{1}{\cos \varphi} \sum_{k=0}^{\infty} \frac{\tan^{2k} \varphi}{2^{2k}} \frac{H_{2k}(x)}{k!}, \quad x \in (-\infty, \infty), \quad |\varphi| \leq \frac{\pi}{4}. \quad (5.18)$$

We differentiate both parts of (5.18) with respect to x and use the formula $H'_n(x) = 2nH_{n-1}(x)$ of the theory of Hermit polynomials [19] and relation (5.17); then, we obtain the expansion of Y in Hermit polynomials:

$$Y \exp\left(\frac{\xi^2}{2}\right) = \frac{\sin^2 2\varphi}{8 \cos^3 \varphi} \sum_{k=0}^{\infty} \frac{\tan^{2k} \varphi}{2^{2k} k!} \frac{H_{2k+1}(\xi)}{k + 1 + \nu/2}, \quad \xi \in (-\infty, \infty), \quad |\varphi| < \frac{\pi}{4}. \quad (5.19)$$

The permissibility of termwise differentiation of (5.18) is justified by absolute convergence of the series of derivatives for $|\varphi| < \pi/4$; this convergence can be established using the asymptotic formulas for Hermit polynomials [19].

Without loss of generality, according to (5.7) the variable φ , irrespective of the signs of the parameters \varkappa and μ , can vary from $-\pi/2$ to $\pi/2$. However, in the case of stagnant cavities under consideration ($U = 0$), the direction of the x axis can be not related to the direction of the mean velocity vector. Provided that the x direction is chosen such that the parameter μ be nonnegative [under the inversion of the x direction, according to (5.1), the signs of \varkappa and μ change to the opposite ones], we can restrict the consideration to the interval $\varphi \in [-\pi/4, \pi/4]$; the end points of the interval correspond to $\mu = 0$. Since relations (5.18) and (5.19) are even with respect to the variable φ , we can restrict the analysis to the interval $\varphi \in (0, \pi/4]$ (recall that the case $\varkappa = 0$ was excluded from the consideration; for this reason, the case $\varphi = 0$ is also excluded). This interval of φ refers to $\varkappa > 0$. Next, we assume that $\varphi \in (0, \pi/4)$; in this case, the series in (5.18) and (5.19) converge.

Using the obtained results (5.14), (5.15), and (5.18), we can derive the following representations of Z in the region of low and high values of the main argument ξ :

$$Z = \frac{\sin^2 2\varphi}{2(2+\nu)} F\left(1, \frac{3}{2}, 2 + \frac{\nu}{2}, \sin^2 \varphi\right) \left\{ \xi + \frac{\xi^3}{6} [3 \cos 2\varphi + 2\nu + 1] \right\} - \frac{\xi^3 \sin^2 2\varphi}{6} + o(\xi^5), \quad \xi \rightarrow 0, \quad (5.20)$$

$$Z = \frac{1}{\xi} \left\{ 1 - \frac{2[\nu + \sin^2 \varphi]}{\xi^2 \sin^2 2\varphi} + O\left(\frac{1}{\xi^4}\right) \right\}, \quad \xi \rightarrow \infty.$$

Here $F(\alpha, \beta, \gamma, z)$ is a hypergeometric function of the listed arguments.

Without loss of generality, the function H in (5.8) can be assumed, as well as Z , an odd function of ξ . Indeed, taking into account relation (5.4) and the structure of Eqs. (5.2), (5.3), and (5.8), we can make the change of the function C by the formula $C = (C_+ + C_-)/2 + C^*$, where the boundary condition over the variable ξ for the new sought function C^* becomes odd-symmetric: $C^* \rightarrow \pm \delta C/2$ for $x \rightarrow \pm\infty$; since C_{\pm} are constant, the general appearance of the equations remains unchanged. For this reason, we assume that the transformation $C \rightarrow C^*$ is accomplished and use the function C^* (or, more precisely, H) as the sought function, omitting the asterisk.

Using the normalization factor A in the expression $H = AW$, with Eq. (5.10) taken into account, we write the equation for W

$$\frac{dW}{d\xi} = 1 - \xi Z, \quad (5.21)$$

which yields, by means of expansions (5.20), the following relations:

$$W = \xi - \frac{\sin^2 2\varphi}{2(2+\nu)} F\left(1, \frac{3}{2}, 2 + \frac{\nu}{2}, \sin^2 \varphi\right) \left\{ \frac{\xi^3}{3} + \frac{\xi^5 [3 \cos 2\varphi + 2\nu + 1]}{30} \right\} + \frac{\xi^5 \sin^2 2\varphi}{30} + o(\xi^7), \quad \xi \rightarrow 0, \quad (5.22)$$

$$W = \frac{1}{2A} - \frac{2[\nu + \sin^2 \varphi]}{\xi \sin^2 2\varphi} + O\left(\frac{1}{\xi^3}\right), \quad \xi \rightarrow \infty.$$

The parameter A in (5.22) will be defined below.

The analog of (5.19) for Z , i.e., the expansion of $W(\xi)$ in Hermit polynomials, obtained by formulas (5.18), (5.19), and (5.21), is

$$W = \frac{Z}{2 \sin^2 \varphi} + \frac{(1+\nu) \exp(-\xi^2 \sin^2 \varphi)}{4 \cos^3 \varphi} \sum_{k=0}^{\infty} \frac{\tan^{2k} \varphi}{2^k} \frac{H_{2k+1}(\xi)}{(2k+1)!!} \sum_{j=0}^k \frac{(2j-1)!!}{2^j (j+1+\nu/2)j!}, \quad (5.23)$$

$$\xi \in (-\infty, \infty), \quad |\varphi| < \pi/4, \quad (2j-1)!! = 3 \cdot 5 \cdot \dots \cdot (2j-1), \quad (-1)!! = 1.$$

The functions $Z(\xi)$ and $W(\xi)$ are plotted for various values of φ and ν in Figs. 2 and 3. In calculating W , it is more convenient to use, instead of (5.23), the numerical integration procedure for Eq. (5.21). From Figs. 2 and 3, it follows that a decrease in φ [see (5.7)] affects the shape of the curves in the same manner as an increase in ν does [see (5.6)]. Curves 2 and 5 in both figures are the same.

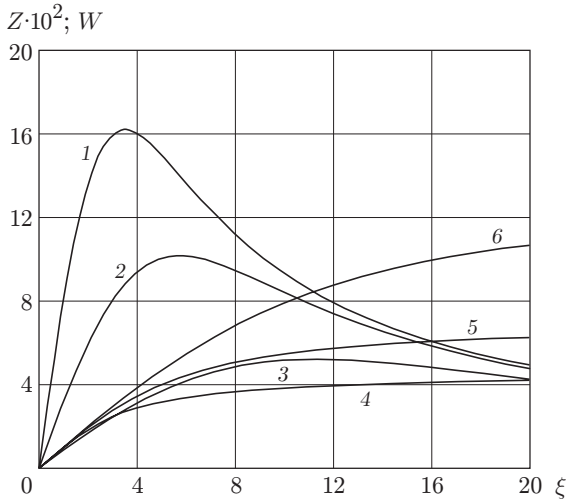


Fig. 2

Fig. 2. Functions $Z(\xi)$ (curves 1–3) and $W(\xi)$ (curves 4–6) for $\nu = 2$ and $\varphi = \pi/7$ (1 and 4), $\pi/12$ (2 and 5), and $\pi/24$ (3 and 6).

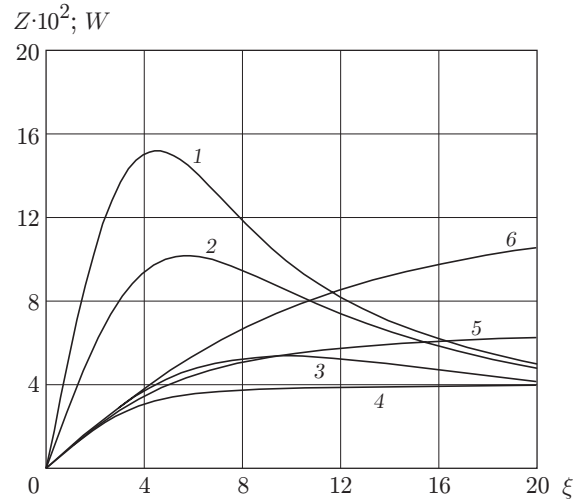


Fig. 3

Fig. 3. Functions $Z(\xi)$ (curves 1–3) and $W(\xi)$ (curves 4–6) for $\varphi = \pi/12$ and $\nu = 0.2$ (1 and 4), 2 (2 and 5), and 10 (3 and 6).

To calculate integral (5.12), we represent the unity in the integrand as $1 = \exp(-\xi^2 \sin^2 \varphi) \exp(\xi^2 \sin^2 \varphi)$ and use expansion (5.18) for $\exp(\xi^2 \sin^2 \varphi)$. The term $\xi Z(\xi)$ in the integrand in (5.12) can also be transformed, with the help of formulas of the theory of Hermit polynomials and using series (5.19), to the expansion in functions $H_{2k}(x)$. As a result, we obtain the expression

$$\begin{aligned} \frac{1}{A} &= \int_{-\infty}^{\infty} [1 - \xi Z(\xi)] d\xi = \frac{\nu + 1}{2 \cos \varphi} \int_{-\infty}^{\infty} \exp(-\xi^2 \sin^2 \varphi) d\xi \sum_{k=0}^{\infty} \frac{\tan^{2k} \varphi}{2^{2k} k!} \frac{H_{2k}(\xi)}{k + 1 + \nu/2} \\ &= \frac{\nu + 1}{2 \cos \varphi} \sum_{k=0}^{\infty} \frac{\tan^{2k} \varphi}{2^{2k} (k + 1 + \nu/2) k!} \int_{-\infty}^{\infty} \exp(-\xi^2 \sin^2 \varphi) H_{2k}(\xi) d\xi \\ &= \frac{\nu + 1}{\sin 2\varphi} \sum_{k=0}^{\infty} \frac{\Gamma(k + 1/2) \Gamma(k + 1 + \nu/2)}{\Gamma(k + 2 + \nu/2) k!} \\ &= \frac{\nu + 1}{\sin 2\varphi} \frac{\Gamma(1/2) \Gamma(1 + \nu/2)}{\Gamma(2 + \nu/2)} F\left(\frac{1}{2}, 1 + \frac{\nu}{2}, 2 + \frac{\nu}{2}, 1\right) = \frac{2\pi \Gamma(1 + \nu/2)}{\Gamma(1/2 + \nu/2) \sin 2\varphi}. \end{aligned}$$

Here the formulas known from the theory of the gamma function and the hypergeometric function are used. The integral of $\exp(-\xi^2 \sin^2 \varphi) H_{2k}(\xi)$ between the infinite limits was calculated in [19]. The permissibility of permutation of integration and summation follows from the absolute convergence, which takes place if $|\varphi| \leq \pi/4$.

Thus, for the mass-transfer coefficient ζ in (5.12) we obtain the expression

$$\zeta = \frac{\sqrt{\alpha D \sin 2\varphi}}{2\pi l} \frac{\Gamma(1/2 + \nu/2)}{\Gamma(1 + \nu/2)}. \quad (5.24)$$

In addition, the expansion of the function W in (5.22) for $\xi \rightarrow \infty$ is now completely determined.

The limiting case ($\nu \rightarrow \infty$ and $\mu \rightarrow 0$) yields the diffusion model of [17]. Using the asymptotic formula for the ratio of gamma-functions for $\nu \rightarrow \infty$ $\Gamma(1/2 + \nu/2)/\Gamma(1 + \nu/2) \cong (2/\nu)^{1/2}$ [19], we obtain

$$\zeta = \alpha \sqrt{D\vartheta} / (\pi l).$$

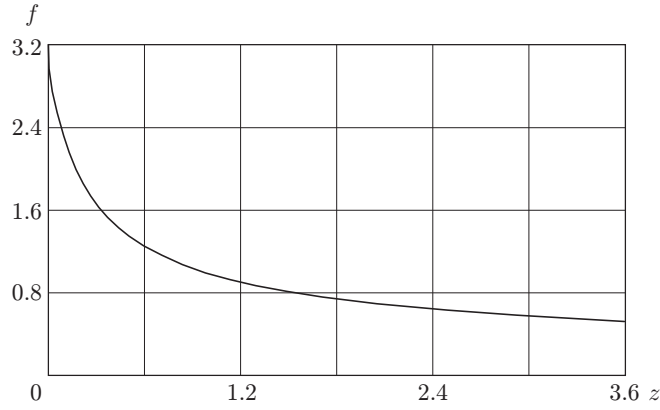


Fig. 4. Function $f(z)$ that describes the mass-transfer coefficient ζ in (5.24).

The function $f(z) = \Gamma(1/4 + z)/\Gamma(3/4 + z)$, which describes the non-elementary part of the mass-transfer coefficient, is plotted in Fig. 4; $z = \nu/2 + 1/4$ and $f = 2\pi l\zeta/[\alpha D \sin 2\varphi]^{1/2}$. From the formulas of the theory of the gamma-function [19], it follows that the function $f(z)$ monotonically decreases with increasing z . Indeed,

$$f'(z) = -f(z) \int_0^1 \frac{x^{z-3/4} dx}{1+x^{1/2}} < 0,$$

since both the integral and the function $f(z)$ are positive in the interval $z \in (0, \infty)$; hence, $f'(z) < 0$ and the function $f(z)$ decreases.

6. System of Several Adjacent Circulation Regions. Provided that the system has several circulation cells with identical parameters, we obtain, following [17], a system of ordinary differential equations for the cell-average concentrations of the substance c_k :

$$\begin{aligned} \frac{dc_1}{d\tau} &= \zeta(c_2 + c_+ - 2c_1), & \frac{dc_N}{d\tau} &= \zeta(c_{N-1} - c_N), \\ \frac{dc_k}{d\tau} &= \zeta(c_{k+1} + c_{k-1} - 2c_k), & k &= 2, 3, \dots, N-1. \end{aligned} \tag{6.1}$$

It is assumed here that the last, N th cell borders on the wall that supplies no substance into the cell, while the substance with some concentration $c_+(\tau)$ enters the first cell; in other words, it can be imagined that there is an additional zeroth cell bordering on the first cell; in the zeroth cell, the concentration is known and varies according to the law $c_+(\tau)$. System (6.1) should be supplemented with the following general initial conditions:

$$c_k \Big|_{\tau=0} = c_k^0, \quad k = 1, 2, \dots, N. \tag{6.2}$$

It is not difficult to extend system (6.1), (6.2) to the case of more complex situations, in which the transfer coefficients ζ can be different at different interfaces between the cells and the interaction of the boundary cells $j = 1$ and $j = N$ with the ambient medium is more complicated.

Conclusions. The main result of the present study is the derivation of system (1.12), (1.13) describing the wave [with zero right sides of (1.12), (1.13)] model with additional conditions (4.4), (4.7)–(4.9). This system extends the results of [5–7] to the case of transfer processes with two-dimensional flows and can be used to analyze natural and technological processes in flow apparatus. In particular, this model may prove useful in analyzing chemical reactors. Simultaneously, the hyperbolic (wave) model includes the diffusion model as a particular case, i.e., this model has a broader field of applicability.

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