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ADMIXTURE DIFFUSION IN A TWO-PHASE RANDOM NONHOMOGENEOUS STRATIFIED LAYER

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Vertical admixture diffusion has been considered in a layer with random nonhomogeneous two-phase stratified structure of the material. Different phase diffusion coefficients and phase densities have been taken into account as well as jump discontinuities of the diffusion coefficient at interphase boundaries. Averaging the obtained expressions for the admixture concentration has been done over the ensemble of sublayer configurations with equally probable distribution, and two particular cases of beta-distribution of phases in the body.
Key words: admixture diffusion, random nonhomogeneous stratified layer

1. Introduction

In practice, often the necessity occurs to describe the process of admixture mass transfer in nonhomogeneous stratified structures. Admixture and behaviour of its distribution in a body have an essential influence on its physical and mechanical properties. The rigorous geometric composition of such structures is unknown, i.e. position and thickness of the sublayers in different materials are random magnitudes. However, their corresponding densities and diffusion coefficients of admixture particles are determined accurately enough.

In certain cases the diffusion coefficients values can differ by some orders of magnitude in different sublayers.

To evaluate the influence of such a structure with substantially different diffusive properties of sublayers on the mass transfer in a body, the methods of homogenisation (Lydzba, 1998; Matysiak and Mieszkowski, 1999) and introduction of effective diffusion coefficients (Kanovsky and Tkachenko, 1991; Lyubov, 1981; Shatinsky and Nesterenko, 1988) has been proposed.

At the study of transfer processes in regular structures, the methods of solving the initial-boundary value problems developed in (Podstrigach et al., 1984) concerning the heat processes can be used.

If the body structure is such that there are macroscopic quantities of particles of different kind sublayers and admixture within an arbitrarily chosen physically small body element, then the continuum-thermodynamical models for description of the diffusion processes (Burak and Chaplia, 1993; Burak et al., 1995) can be also used.

However, the cases have been described in literature (Lyubov, 1981; Kanovsky and Tkachenko, 1991) when introduction of an effective diffusion coefficient and experimental data interpretation on this basis are not always physically justified. But we can make certain reliable assumptions concerning the stochastic distribution of sublayers in the body.

2. Problem formulation

Let the admixture particles migrate in a dispersed layer of thickness z_0 with randomly nonhomogeneous stratified structure of material. The body is composed of two solid phases with different densities (Fig. 1), and admixture diffusion coefficients can differ essentialy in these phases. The discussion is restricted to the case when the volume fraction v_0 of one phase (the basic phase, marked by the index 0) is much greater than that of another phase $v_0 \gg v_1$.

If an arbitrary vertical body volume is denoted by V then $V = V^{(0)} + V^{(1)}$, where $V^{(j)}$ is the volume of the j-phase, and

$$V^{(j)} = \bigcup_{i=1}^{n_j} V_i^{(j)} \qquad\qquad j = 0; 1$$

Here $V_i^{(j)}$ is the volume of sublayer i of the j-phase, i is the sublayer number, $i = 1, 2, ..., n_j$, n_j is the number of sublayers of kind j. And we assume that

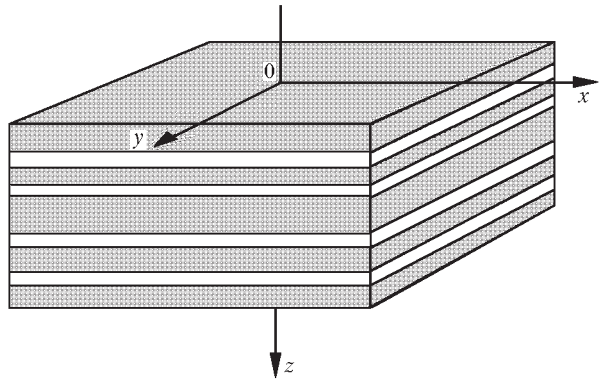

Fig. 1. One of possible realizations of the body structure

the body density $\rho(z)$ and diffusion coefficient $D(z)$ are constant in the volume of each phase. At the same time, the phase configuration is a random magnitude.

Let us introduce into consideration the random operator $\eta_{ij}(z)$ that depends on the phase configuration and doesn't depend on their physical characteristics. It is defined by the formula (Lydzba, 1998)

$$\eta_{ij}(z) = \begin{cases} 1 & z \in V_i^{(j)} \\ 0 & z \notin V_i^{(j)} \end{cases} \tag{2.1}$$

Note that

$$\sum_{j=0}^{1} \sum_{i=1}^{n_j} \eta_{ij}(z) = 1 \tag{2.2}$$

Relationship (2.2) represents the body continuity.

Then the diffusion coefficient $D(z)$ and density of the body $\rho(z)$ are presented by the random operator (2.1) as follows

$$D(z) = \sum_{j=0}^{1} \sum_{i=1}^{n_j} D_j \eta_{ij}(z) \qquad\qquad \rho(z) = \sum_{j=0}^{1} \sum_{i=1}^{n_j} \rho_j \eta_{ij}(z) \tag{2.3}$$

where D_j, ρ_j are values of the corresponding coefficients in j-phase.

Using the approach of generalized functions (Vladimirov, 1976; Podstrigach et al., 1984), diffusion of admixture particles in such a body is described in the form

$$L(z,t)c(z,t) \equiv \overline{\rho}(z)\frac{\partial c(z,t)}{\partial t} - \nabla[D(z)\nabla c(z,t)] = 0 \tag{2.4}$$

where $c(z,t)$ denotes the field of admixture concentration in the body; $\overline{\rho}(z) = \rho(z)/\rho_0$ is the normalized random density and $\rho(z)$ is the body density, ρ_0 is the density of the phase 0; $D(z)$ is a random admixture diffusion coefficient, $D(z) = d(z)/\rho_0$, and here $d(z)$ is a random kinetic coefficient; $\nabla = \partial/\partial z$, t is time.

Let a constant mass source act on the upper boundary of the layer referred to rectangular coordinates so that the Oz-axis is perpendicular to its surface $z = 0$

$$c(z,t)|_{z=0} = c^* \qquad\qquad (c^* = \text{const})$$

Another boundary condition and the initial one are also given

$$c(z,t)|_{z=z_0} = 0 \qquad\qquad c(z,t)|_{t=0} = 0 \tag{2.5}$$

Substitute the coefficient (2.3) into Eq. (2.4) and assume that (Vladimirov, 1974)

$$\sum_{j=0}^{1}\sum_{i=1}^{n_j} \nabla\Big(D_j\eta_{ij}(z)\Big) = \sum_{j=0}^{1}\sum_{i=1}^{n_j}[D_j]_\Gamma\delta(z - z_{ij}^\Gamma)$$

where $[D_j]_\Gamma$ denotes a jump of the diffusion coefficient on the boundaries of the i-layer of the j-phase $(V_i^{(j)})$, $\delta(z)$ is the Dirac delta-function, z_{ij}^Γ is the boundary of subregion $V_i^{(j)}$ (henceforth z_{ij} denotes the upper boundary of $V_i^{(j)}$ (random magnitude); $z_{ij} + \delta z_j$ is the lower boundary of this sublayer, δz_j is the width of the j-phase layer). Then we obtain

$$L(z,t)c(z,t) = \sum_{j=0}^{1}\sum_{i=1}^{n_j} L_{ij}(z,t)c(z,t) = 0 \tag{2.6}$$

where the random operator L_{ij} is

$$\begin{aligned} L_{ij}(z,t) = \overline{\rho}_j\eta_{ij}(z)\frac{\partial}{\partial t} - D_j\eta_{ij}(z)\frac{\partial^2}{\partial z^2} - \\ -\Big[[D_j]_\Gamma^h\delta(z - z_{ij}) + [D_j]_\Gamma^l\delta(z - (z_{ij} + \delta z_j))\Big]\frac{\partial}{\partial z} \end{aligned}$$

Here $[D_j]_\Gamma^h$, $[D_j]_\Gamma^l$ are jumps of the diffusion coefficient on the upper and lower boundaries of the i-sublayer of the j-phase (random magnitude).

3. Neyman series for the diffusion problem

In Eq. (2.6) add and subtract deterministic operator $L_0(z,t)$ defined in the entire interval $(t \in [0;\infty[,\ z \in [0;z_0])$

$$L_0(z,t) = \overline{\rho}_0 \frac{\partial}{\partial t} - D_0 \frac{\partial^2}{\partial z^2}$$

the coefficients of which are characteritics of the basic phase. Then using conditions (2.2) we have

$$L_0(z,t)c(z,t) = L_s(z,t)c(z,t) \tag{3.1}$$

where

$$\begin{aligned} L_s(z,t) \equiv L_0 - L = \overline{\rho}_* \sum_{i=1}^{n_1} \eta_{i1}(z) \frac{\partial}{\partial t} - D_* \sum_{i=1}^{n_1} \eta_{i1}(z) \frac{\partial^2}{\partial z^2} + \\ + D_* \sum_{i=1}^{n_1} \Big[\delta(z - z_{i1}) - \delta(z - (z_{i1} + \delta z_1)) \Big] \frac{\partial}{\partial z} \end{aligned} \tag{3.2}$$

Here $\overline{\rho}_* = \overline{\rho}_0 - \overline{\rho}_1$ and $D_* = D_0 - D_1$. We consider the right-hand side of Eq. (3.1) as a source, i.e. the medium nonhomogeneity is treated as internal source. The solution of initial-boundary value problem (3.1), (2.5) is found in the form of Neyman series (Rytov et al., 1978).

Let $c_0(z,t)$ by a deterministic field of admixture concentration in the body with characteristics $\overline{\rho}_0$, D_0. It satisfies the following homogeneous equation

$$L_0(z,t)c_0(z,t) = 0$$

and the initial boundary conditions (2.5), i.e. (Crank, 1975)

$$c_0(z,t) = c^* \Big\{ 1 - \frac{z}{z_0} - \sum_{n=1}^{\infty} \frac{2}{n\pi} \exp\Big(-\frac{D_0}{\overline{\rho}_0} y_n^2 t \Big) \sin(y_n z) \Big\} \tag{3.3}$$

where $y_n = n\pi/z_0$.

Write $G(z,z',t,t')$ for the unperturbed Green function satisfying a diffusion equation for a point source

$$\overline{\rho}_0 \frac{\partial G}{\partial t} - D_0 \frac{\partial^2 G}{\partial z^2} = \delta(t - t')\delta(z - z')$$

and the initial and boundary conditions

$$G(z, z', t, t')|_{t=0} = 0$$
$$G(z, z', t, t')|_{z=0} = G(z, z', t, t')|_{z=z_0} = 0$$

Then the initial-boundary value problem (3.1), (2.5) is equivalent to the integral equation for the random field of admixture concentration $c(z,t)$ in a two-phase stratified layer

$$c(z,t) = c_0(z,t) + \int_0^t \int_0^{z_0} G(z, z', t, t') L_s(z', t') c(z', t')\, dz' dt' \tag{3.4}$$

where the Green function is

$$G(z, z', t, t') = \frac{1}{2\overline{\rho}_0} \sum_{n=1}^{\infty} \exp\Big[-\frac{D_0}{\overline{\rho}_0} y_n^2 (t-t')\Big] \Big[\cos(y_n(z-z')) - \cos(y_n(z+z'))\Big] \tag{3.5}$$

The Neyman series for the problem (3.1), (2.5) is built by iterating (Rytov at al., 1978) the integral equation (3.4). Let us restrict the expression to the first two terms in the Neyman series. Then we obtain

$$c(z,t) \approx c_0(z,t) + \int_0^t \int_0^{z_0} G(z, z', t, t') L_s(z', t') c_0(z', t')\, dz' dt' \tag{3.6}$$

If we substitute the operator $L_s(z', t')$ defined by (3.2) into Eq. (3.6), we have

$$\begin{aligned} c(z,t) \approx c_0(z,t) &+ \int_0^t \int_0^{z_0} G(z, z', t, t') \sum_{n=1}^{\infty} \Big[\overline{\rho}_* \frac{\partial c_0}{\partial t'} - D_* \frac{\partial^2 c_0}{\partial z'^2}\Big] \eta_{i1}(z')\, dz' dt' + \\ &+ D_* \int_0^t \int_0^{z_0} G(z, z', t, t') \sum_{n=1}^{\infty} \Big[\delta(z' - z_{i1}) - \delta(z' - (z_{i1} + \delta z_1))\Big] \frac{\partial c_0}{\partial z'}\, dz' \end{aligned} \tag{3.7}$$

4. Averaging approximate solution

Let us consider averaging of the concentration field over the ensemble of sublayer configurations with different distributions of phases in the body.

I. Let the phases be distributed with equal probabilities. As $c_0(z,t)$ is a deterministic field, then $\langle c_0(z,t)\rangle_{conf} = c_0(z,t)$. Consider the first integral in (3.7). As long as

$$\eta_{i1}(z') = \begin{cases} 1 & z' \in [z_{i1}; z_{i1}+\delta z_1] \\ 0 & z \notin [z_{i1}; z_{i1}+\delta z_1] \end{cases} = \begin{cases} 1 & z'-z_{i1} \in [0;\delta z_1] \\ 0 & z'-z_{i1} \notin [0;\delta z_1] \end{cases} = \eta_{i1}(z'-z_{i1}) \tag{4.1}$$

only the function $\eta_{i1}(z'-z_{i1})$ depends on z_{i1} under the integral and there are not other terms with index i, then

$$\langle I_1\rangle_{conf} = \int\limits_0^t \int\limits_0^{z_0} G(z,z',t,t')L_*(z',t')c_0(z',t')\frac{1}{V}\sum_{i=1}^{n_j}\int\limits_V \eta_{i1}(z'-z_{i1})\, dz_{i1}dz'dt'$$

$$L_*(z',t') = \overline{\rho}_*\frac{\partial}{\partial t'} - D_*\frac{\partial^2}{\partial z'^2}$$

Taking into account the properties of function $\eta_{i1}(z'-z_{i1})$, we can write

$$\frac{1}{V}\sum_{i=1}^{n_j}\int\limits_V \eta_{i1}(z'-z_{i1})dz_{i1} = \begin{cases} v_1\dfrac{z'}{\delta z_1} & z' < \delta z_1 \\ v_1 & z' \geqslant \delta z_1 \end{cases}$$

Then we obtain

$$\langle I_1\rangle_{conf} = \frac{v_1}{\delta z_1}\int\limits_0^t\int\limits_0^{\delta z_1} GL_*c_0(z',t')z'\, dz'dt' + v_1\int\limits_0^t\int\limits_{\delta z_1}^{z_0} GL_*c_0(z',t')\, dz'dt' \tag{4.2}$$

Consider averaging of the second integral in (3.7). Since the δ-function is even, we have (Abramowitz and Stegun, 1979)

$$\int\limits_0^{z_0-\delta z_1} \delta(z_{i1}-z')\, dz_{i1} = \begin{cases} \dfrac{1}{2} & z'=0 \quad \text{or} \quad z'=z_0-dz_1 \\ 1 & z' \in]0; z_0-\delta z_1[\\ 0 & \text{for other } z' \end{cases}$$

and

$$\frac{1}{V}\sum_{i=1}^{n_j}\int\limits_V \delta(z_{i1}-z')\, dz_{i1} = \begin{cases} \dfrac{v_1}{2\delta z_1} & z'=0 \quad \text{or} \quad z'=z_0-\delta z_1 \\ \dfrac{v_1}{\delta z_1} & z' \in]0; z_0-\delta z_1[\\ 0 & \text{for other } z' \end{cases} \tag{4.3}$$

We find the internal integral of the second δ-function in the same way

$$\frac{1}{V}\sum_{i=1}^{n_j}\int_V \delta(z_{i1}+\delta z_1 - z')\,dz_{i1} = \begin{cases} \dfrac{v_1}{2\delta z_1} & z'=\delta z_1 \quad \text{or} \quad z'=z_0 \\ \dfrac{v_1}{\delta z_1} & z' \in]\delta z_1; z_0[\\ 0 & \text{for other } z' \end{cases} \tag{4.4}$$

Then, allowing for (4.3), (4.4), the definition of an improper integral, the boundary conditions for the Green function, we obtain

$$\begin{gathered} \langle I_2\rangle_{conf} = D_* \frac{v_1}{\delta z_1}\int_0^t \Big\{\frac{1}{2}\Big(G\frac{\partial c_0}{\partial z'}\Big|_{z'=z_0-\delta z_1} - G\frac{\partial c_0}{\partial z'}\Big|_{z'=\delta z_1}\Big) + \\ + \int_{+0}^{\delta z_1+0} G\frac{\partial c_0}{\partial z'}\,dz' - \int_{z_0-\delta z_1+0}^{z_0-0} G\frac{\partial c_0}{\partial z'}\,dz'\Big\}\,dt' \end{gathered} \tag{4.5}$$

As long as (4.2) and (4.5) take place, we can write the expression for calculating the approximate concentration field averaged over the ensemble of sublayer configurations

$$\begin{gathered} \langle c\rangle_{conf} = c_0(z,t) + \frac{v_1}{\delta z_1}\int_0^t \Big\{\int_0^{\delta z_1} GL_* c_0(z',t') z'\,dz' + \\ +\delta z_1 \int_{\delta z_1}^{z_0} GL_* c_0(z',t')\,dz' + D_*\Big[\frac{1}{2}\Big(G\frac{\partial c_0}{\partial z'}\Big|_{z'=z_0-\delta z_1} - G\frac{\partial c_0}{\partial z'}\Big|_{z'=\delta z_1}\Big) + \\ + \int_{+0}^{\delta z_1+0} G\frac{\partial c_0}{\partial z'}\,dz' - \int_{z_0-\delta z_1+0}^{z_0-0} G\frac{\partial c_0}{\partial z'}\,dz'\Big]\Big\}\,dt' \end{gathered} \tag{4.6}$$

II. Let the phase $j=1$ have the beta-distribution in the layer. Note that the density of the beta-distribution in a layer with thickness z_0 is

$$f(z) = \begin{cases} \dfrac{\Gamma(\alpha+\beta)}{\Gamma(\alpha)\Gamma(\beta)}\Big(\dfrac{z}{z_0}\Big)^{\alpha-1}\Big(1-\dfrac{z}{z_0}\Big)^{\beta-1} & z\in[0;z_0] \\ 0 & z\notin[0;z_0] \quad (\alpha>0,\ \beta>0) \end{cases}$$

Below we consider two special cases: (i) $\alpha>1$, $\beta=1$; (ii) $\alpha=1$, $\beta>1$ (Fig. 2).

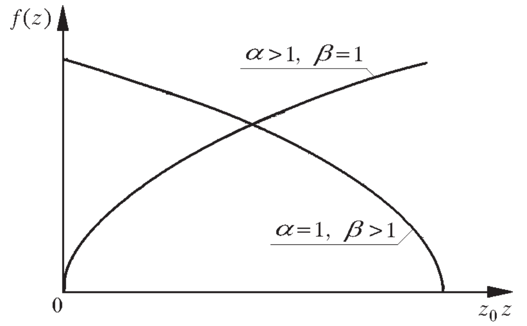

Fig. 2. Density of beta-distribution

Let us average the concentration field over the ensemble of sublayer configurations (3.7) with the beta-distribution of the phase $j = 1$. For this purpose consider the averaging of the first integral in (3.7)

$$\langle I_1 \rangle_{conf} = \int_0^t \int_0^{z_0} GL_* c_0(z', t') \sum_{i=1}^{n_j} \int_V \eta_{i1}(z') f(z_{i1})\, dz_{i1} dz' dt'$$

(i) Taking into account the expression for $f(z)$, in this case we have

$$\sum_{i=1}^{n_j} \int_V \eta_{i1}(z') f(z_{i1})\, dz_{i1} = \frac{\Gamma(1+\alpha)}{\Gamma(\alpha)} \sum_{i=1}^{n_j} \int_0^{z_0 - \delta z_1} \eta_{i1}(z' - z_{i1}) \Big(\frac{z_{i1}}{z_0 - \delta z_1} \Big)^{\alpha - 1} dz_{i1}$$

Using (4.1) we obtain two cases: if $z' < \delta z_1$ then

$$\sum_{i=1}^{n_j} \int_V \eta_{i1}(z') f(z_{i1})\, dz_{i1} = \frac{\Gamma(1+\alpha)}{\alpha \Gamma(\alpha)} \frac{v_1 (z')^\alpha}{\delta z_1 (z_0 - \delta z_1)^{\alpha - 2}}$$

When $z' \geqslant \delta z_1$

$$\sum_{i=1}^{n_j} \int_V \eta_{i1}(z') f(z_{i1})\, dz_{i1} = \frac{\Gamma(1+\alpha)}{\alpha \Gamma(\alpha)} \frac{v_1 [(z')^\alpha - (z' - \delta z_1)^\alpha]}{\delta z_1 (z_0 - \delta z_1)^{\alpha - 2}}$$

In consequence, we obtain

$$\langle I_1 \rangle_{conf} = \frac{\Gamma(1+\alpha)}{\alpha \Gamma(\alpha)} \frac{v_1}{\delta z_1} (z_0 - \delta z_1)^{2-\alpha} \cdot$$

$$\cdot \int_0^t \Big\{ \int_0^{\delta z_1} {z'}^\alpha GL_* c_0(z', t')\, dz' - \int_{\delta z_1}^{z_0} (z' - \delta z_1)^\alpha GL_* c_0(z', t')\, dz' \Big\} dt'$$

(ii) Using the expression of the beta-distribution density when $\alpha = 1$, $\beta > 1$, we have

$$\sum_{i=1}^{n_j} \int_V \eta_{i1}(z') f(z_{i1})\, dz_{i1} = \frac{\Gamma(1+\beta)}{\Gamma(\beta)} \sum_{i=1}^{n_j} \int_0^{z_0-\delta z_1} \eta_{i1}(z'-z_{i1}) \Big(1 - \frac{z_{i1}}{z_0-\delta z_1}\Big)^{\beta-1} dz_{i1}$$

Integrating the last expression we obtain

$$\langle I_1 \rangle_{conf} = \frac{\Gamma(1+\beta)}{\beta\Gamma(\beta)} \frac{v_1}{\delta z_1} (z_0-\delta z_1)^{2-\beta} \int_0^t \Big\{ \int_{\delta z_1}^{z_0} (z_0 - z')^{\beta} G L_* c_0(z',t')\, dz' -$$

$$- \int_0^{z_0} (z_0 - \delta z_1 - z')^{\beta} G L_* c_0(z',t')\, dz' + (z_0-\delta z_1)^{\beta} \int_0^{\delta z_1} G L_* c_0(z',t')\, dz' \Big\}\, dt'$$

Since the Dirac function is an even one, the averaged second integral in (3.7) can be written in the form:

(i)

$$\langle I_2 \rangle_{conf} = D_* \frac{\Gamma(1+\alpha)}{\Gamma(\alpha)} \frac{v_1}{\delta z_1} (z_0-\delta z_1)^{2-\alpha} \int_0^t \int_0^{z_0} G L_* c_0(z',t') \cdot$$

$$\cdot \Big({z'}^{\alpha-1} - (z'-\delta z_1)^{\alpha-1} \Big)\, dz' dt'$$

(ii)

$$\langle I_2 \rangle_{conf} = D_* \frac{\Gamma(1+\beta)}{\Gamma(\beta)} \frac{v_1}{\delta z_1} (z_0-\delta z_1)^{2-\beta} \int_0^t \int_0^{z_0} G L_* c_0(z',t') \cdot$$

$$\cdot \Big((z_0 - \delta z_1 - z')^{\beta-1} - (z_0-\delta z_1)^{\beta-1} \Big)\, dz' dt'$$

As a result we obtain the formulae for the admixture concentration field averaged over the ensemble of sublayer configurations with their beta-distribution:

(i)

$$\langle c \rangle_{conf} = c_0(z,t) + \frac{\Gamma(1+\alpha)}{\Gamma(\alpha)} \frac{v_1}{\delta z_1} \Big(z_0 - \delta z_1\Big)^{2-\alpha} \int_0^t \Big\{ \frac{1}{\alpha} \int_0^{\delta z_1} {z'}^{\alpha} G L_* c_0(z',t') dz' -$$

$$- \frac{1}{\alpha} \int_{\delta z_1}^{z_0} (z'-\delta z_1)^{\alpha} G L_* c_0(z',t') dz' + D_* \int_0^{z_0} G \frac{\partial c_0}{\partial z'} \Big[{z'}^{\alpha-1} - (z'-\delta z_1)^{\alpha-1} \Big] dz' \Big\} dt' \qquad (4.7)$$

(ii)

$$\langle c\rangle_{conf} = c_0 + \frac{\Gamma(1+\beta)}{\Gamma(\beta)}\frac{v_1}{\delta z_1}\Big(z_0-\delta z_1\Big)^{2-\beta}\int_0^t\Big\{\frac{1}{\beta}\int_{\delta z_1}^{z_0}(z_0-z')^\beta GL_* c_0(z',t')dz' -$$
$$-\frac{1}{\beta}\int_0^{z_0}(z_0-z'-\delta z_1)^\beta GL_* c_0(z',t')dz' + \frac{1}{\beta}(z_0-\delta z_1)^\beta\int_0^{\delta z_1} GL_* c_0(z',t')dz' + \tag{4.8}$$
$$+D_*\int_0^{z_0} G\frac{\partial c_0}{\partial z'}\Big[(z_0-z'-\delta z_1)^{\beta-1}-(z_0-\delta z_1)^{\beta-1}\Big]dz'\Big\}dt'$$

5. Analysis of the obtained solutions

The final expression for the averaged field of the admixture concentration for different distributions of sublayers in the two-phase stratified layer is obtained by substituting the formulae for the Green function and the admixture concentration in the homogeneous medium with characteristics of the phase $j = 0$ into the respective expressions for the averaged concentration fields.

I. The equally probable distribution of the phases. Substituting Eqs (3.3) and (3.5) into (4.6) we have

$$\frac{1}{c^*}\langle c(z,t)\rangle_{conf} = 1-\frac{z}{z_0}-\sum_{n=1}^{\infty}\frac{2}{n\pi}\exp\Big(-\frac{D_0}{\overline{\rho}_0}y_n^2 t\Big)\sin(y_n z)+$$
$$+\frac{v_1}{\delta z_1}\frac{D_*}{2z_0 D_0}\Big\{\delta z_1(z_0-2z)+\sum_{k=1}^{\infty}\frac{1}{y_k}\exp\Big(-\frac{D_0}{\overline{\rho}_0}y_k^2 t\Big)\Big[\Big(B_1+\frac{1}{y_k}B_2\Big)\cos(y_k\delta z_1)-$$
$$-B_2 z_0\sin(y_k\delta z_1)\Big]+\sin(y_k z)\Big[\frac{D_*}{y_k^3}(1-(-1)^k)(1-\cos(y_k\delta z_1))+ \tag{5.1}$$
$$+\sum_{n=1}^{\infty}\frac{1}{y_n^2-y_k^2}\Big[\exp\Big(-\frac{D_0}{\overline{\rho}_0}y_k^2 t\Big)-\exp\Big(-\frac{D_0}{\overline{\rho}_0}y_n^2 t\Big)\Big]\cdot$$
$$\cdot\Big(2\frac{D_\rho}{D_*}y_n(A_- - A_+)-(1+(-1)^{k+n})A_{kn}\Big)\Big]\Big\}$$

where

$$B_1 = 2\sin(y_k\delta z_1)\cos(y_k z) \qquad B_2 = 2\cos(y_k\delta z_1)\cos(y_k z)$$

$$D_\rho = \frac{D_1\overline{\rho}_0 - D_0\overline{\rho}_1}{\overline{\rho}_0} \qquad A_\pm = \frac{1}{(y_k \pm y_n)^2}[\cos((y_k \pm y_n)\delta z_j) - 1]$$

$$A_{kn} = \frac{2y_k}{y_k^2 - y_n^2} - \frac{\cos[(y_k - y_n)\delta z_1]}{y_k - y_n} - \frac{\cos[(y_k + y_n)\delta z_1]}{y_k + y_n}$$

Illustration of the influence of the material structure nonhomogeneity on the distribution of the admixture concentration in a layer under the action of a constant source on the upper boundary is given in Fig. 3 and Fig. 4. Numerical calculation was done for the dimensionless quantities $\xi = z/z_0$ and $\mathrm{Fo} = D_0 t/z_0^2$. It is assumed that $\overline{D}_1 = D_1/D_0 = 0.5$, $\delta\xi_1 = \delta z_1/z_0 = 0.01$, $\mathrm{Fo} = 10^{-2}$, $v_1 = 0.1$. The solid line marks the respective function for the admixture concentration averaged over the ensemble of sublayer configurations and calculated by (5.1). The dashed line identifies the admixture concentration in the homogeneous medium with the basic phase characteristics. The dimensionless coordinate ξ has been assumed as abscissa, the ratio of the concentration to its value on the upper body boundary c^* has been taken as ordinate. The distributions of the admixture concentration are compared in Fig. 3a for different values of the reduced diffusion coefficient $\overline{D}_1 = 0.2$, 0.5, 0.8, 1.2, 1.5, curves 1-5, respectively. The concentration distributions are presented for different values of the Fourier number $\mathrm{Fo} = 10^{-2}$, 10^{-3}, 10^{-4}, curves 1-3 ($1a - 3a$) respectively, in Fig. 3b.

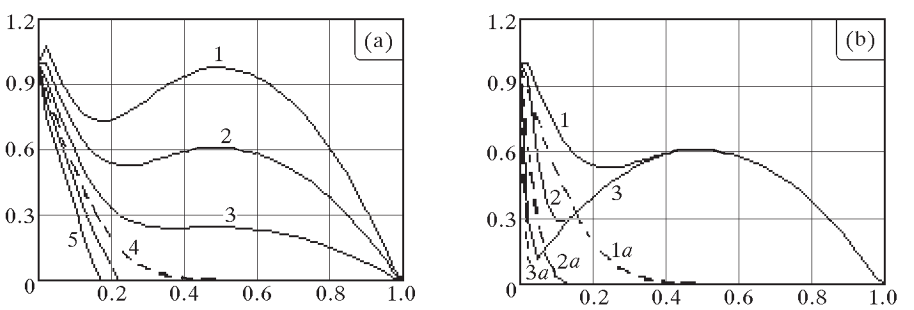

Fig. 3.

Fig. 4a illustrates the behaviour of the concentration field in dependence on the quantity of the volume fraction of sublayers $v_1 = 0.2$, 0.15, 0.1, 0.05, 0.01, curves 1-5, respectively. Dependence of the admixture concentration on the sublayer thickness $\delta\xi_1 = 0.05$, 0.02, 0.01, 0.008, 0.007, curves 1-5, is shown in Fig. 4b.

The performed analysis of the obtained results shows that distinctions in diffusive properties of the randomly distributed phases can cause essential

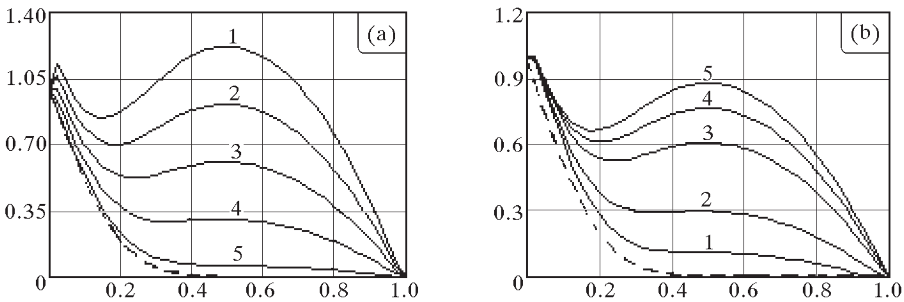

Fig. 4.

changes of the character of the admixture concentration field in the body. Thus in quantitative description of the mass transfer it is necessary to take into account explicitly both different values of the diffusion coefficient and its jump discontinuities at phase boundaries. In the case when the diffusion coefficient in thin layers is greater than the one in the matrix, it leads the admixture concentration decrease in the body. And occurence of sublayers with the diffusion coefficient smaller than one in the matrix causes its essential increase (Fig. 3a).

Change of the other material parameters affects also substantially the values of the averaged concentration field in a nonhomogeneous medium. Thus, in the case of the admixture diffusion in bodies with $\overline{D}_1 < \overline{D}_0$, increase of the sublayer volume fraction causes increase of the averaged concentration, both near the body surface and in the middle region of the layer (Fig. 4a). And increasing the layer thickness at the same sublayer volume fraction decreases the admixture concentration in the body (Fig. 4b). Note that homogenized models can be used for description of diffusion processes in small time intervals.

II. The beta-distritution of sublayers

(i) To obtain the expression of the averaged concentration field in this case, we substitute the formulae (3.3) and (3.5) into (4.7)

$$\frac{1}{c^*}\langle c(z,t)\rangle_{conf} = 1 - \frac{z}{z_0} - \sum_{n=1}^{\infty} \frac{2}{n\pi} \exp\Big(-\frac{D_0}{\overline{\rho}_0} y_n^2 t\Big) \sin(y_n z) +$$
$$+ \frac{\Gamma(1+\alpha)}{\Gamma(\alpha)} \frac{v_1}{\delta z_1} \frac{(z_0 - \delta z_1)^{2-\alpha}}{z_0 D_0} \sum_{k=1}^{\infty} \sin(y_k z) \Big\{ \frac{D_*}{2y_k^2} \Big[\exp\Big(-\frac{D_0}{\overline{\rho}_0} y_k^2 t\Big) - 1 \Big] \cdot$$
$$\cdot \Big[f_s^{\alpha-1}(0, z_0, 0, y_n) - f_s^{\alpha-1}(0, z_0, \delta z_1, y_n) \Big] +$$

$$
\begin{aligned}
&+\sum_{n=1}^{\infty}\frac{1}{y_n^2-y_k^2}\Big[\exp\Big(-\frac{D_0}{\overline{\rho}_0}y_k^2t\Big)-\exp\Big(-\frac{D_0}{\overline{\rho}_0}y_n^2t\Big)\Big]\cdot\\
&\cdot\Big\{\frac{1}{\alpha}D_\rho y_n\Big[f_c^\alpha(0,\delta z_1,0,y_k-y_n)-f_c^\alpha(0,\delta z_1,0,y_k+y_n)-\\
&-f_c^\alpha(\delta z_1,z_0,\delta z_1,y_k-y_n)+f_c^\alpha(\delta z_1,z_0,\delta z_1,y_k+y_n)\Big]-\\
&-\frac{1}{2}D_*\Big[f_s^{\alpha-1}(0,z_0,0,y_k-y_n)+f_s^{\alpha-1}(0,z_0,0,y_k+y_n)-\\
&-f_s^{\alpha-1}(0,z_0,\delta z_1,y_k-y_n)-f_s^{\alpha-1}(0,z_0,\delta z_1,y_k+y_n)\Big]\Big\}\Big\}
\end{aligned}
\tag{5.2}
$$

where

$$
f_s^\alpha(a,b,c,d)=\int_a^b(z-c)^\alpha\sin(zd)\,dz
$$

$$
f_c^\alpha(a,b,c,d)=\int_a^b(z-c)^\alpha\cos(zd)\,dz
$$

(ii) Substituting (3.3) and (3.5) into (4.8) we obtain the expression for the averaged concentration field in the layer with the beta-distribution of sublayers when $\alpha=1,\ \beta>1$

$$
\begin{aligned}
&\frac{1}{c^*}\langle c(z,t)\rangle_{conf}=1-\frac{z}{z_0}-\sum_{n=1}^{\infty}\frac{2}{n\pi}\exp\Big(-\frac{D_0}{\overline{\rho}_0}y_n^2t\Big)\sin(y_nz)+\\
&+\frac{\Gamma(1+\beta)}{\Gamma(\beta)}\frac{v_1}{\delta z_1}\frac{(z_0-\delta z_1)^{2-\beta}}{z_0D_0}\Big\{D_*\frac{zz_0}{8}\Big(1-\frac{z}{z_0}\Big)(z_0-\delta z_1)^{\beta-1}+\\
&+\sum_{k=1}^{\infty}\sin(y_kz)\Big\{\frac{D_*}{2}\Big[\frac{1}{y_k^2}f_s^{\beta-1}(-z_0,0,\delta z_1-z_0,y_k)\Big[1-\exp\Big(-\frac{D_0}{\overline{\rho}_0}y_k^2t\Big)\Big]-\\
&-(z_0-\delta z_1)^{\beta-1}(1-(-1)^k)\Big(\frac{1}{y_k^2}-1\Big)\frac{1}{y_k}\exp\Big(-\frac{D_0}{\overline{\rho}_0}y_k^2t\Big)\Big]+\\
&+\sum_{n=1}^{\infty}\frac{1}{y_n^2-y_k^2}\Big[\exp\Big(-\frac{D_0}{\overline{\rho}_0}y_k^2t\Big)-\exp\Big(-\frac{D_0}{\overline{\rho}_0}y_n^2t\Big)\Big]\Big[\frac{D_\rho}{2\beta}y_nA(z_0-\delta z_1)^\beta-\\
&-\frac{D_\rho}{\beta}y_n\Big[f_c^\alpha(-z_0,0,\delta z_1-z_0,y_k-y_n)-f_c^\alpha(-z_0,0,\delta z_1-z_0,y_k+y_n)+
\end{aligned}
\tag{5.3}
$$

$$+f_c^{\alpha}(-z_0,-\delta z_1,-z_0,y_k-y_n)-f_c^{\alpha}(-z_0,-\delta z_1,-z_0,y_k+y_n)\Big]-$$
$$-\frac{1}{2}D_*\Big[f_s^{\beta-1}(-z_0,0,\delta z_1-z_0,y_k-y_n)+f_s^{\beta-1}(-z_0,0,\delta z_1-z_0,y_k+y_n)]\Big]-$$
$$-D_*y_k\sum_{n=1}^{\infty}\frac{1-(-1)^{k+n}}{y_n^2-y_k^2}\exp\Big(-\frac{D_0}{\overline{\rho}_0}y_n^2t\Big)\Big\}\Big\}$$

where

$$A=\frac{\sin(y_k-y_n)\delta z_1}{y_k-y_n}-\frac{\sin(y_k+y_n)\delta z_1}{y_k+y_n}$$

The distributions of the admixture concentration field in a stratified layer is given in Fig. 5 and Fig. 6 for the particular cases of the probable beta-distribution of sublayers. Numerical calculation was also done for the dimensionless quantities $\xi = z/z_0$ and $\mathrm{Fo} = D_0t/z_0^2$. Then we assume $\overline{D}_1 = D_1/D_0 = 0.5$, $\delta\xi_1 = \delta z_1/z_0 = 0.01$, $\mathrm{Fo} = 10^{-1}$, $v_1 = 0.1$. The dashed line (curves *a*) marks the respective function for admixture concentration averaged over the ensemble of sublayers configurations with their beta-distribution in the body for the case $\alpha > 1, \beta = 1$ and calculated by (5.2). The solid line (curves *b*) identifies the admixture concentration for the case $\alpha = 1$, $\beta > 1$ and calculated by the expression (5.3). The dimensionless coordinate ξ has been assumed as abscissa, the ratio of the concentration to its value on the upper body boundary c^* has been assumed as ordinate. The distributions of the admixture concentration are compared in Fig. 5a for different values of the reduced diffusion coefficient $\overline{D}_1 = 0.2, 0.5, 0.8, 1.2, 1.5$, curves 1-5, respectively. The concentration distributions are presented for different values of Fourier number $\mathrm{Fo} = 10^{-1}, 5\cdot 10^{-2}, 10^{-2}$, curves 1-3 respectively, in Fig. 5b.

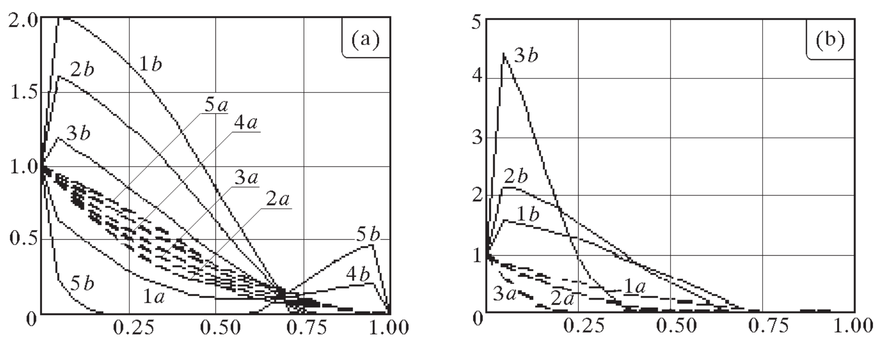

Fig. 5.

Fig. 6a illustrates the behaviour of the concentration field in dependence on the quantity of the volume fraction of sublayers $v_1 = 0.2, 0.15, 0.1, 0.05, 0.01$, curves 1-5, respectively. Dependence of the admixture concentration on the sublayer thickness $\delta\xi_1 = 0.05, 0.02, 0.01, 0.008$, curves 1-4, is shown in Fig. 6b.

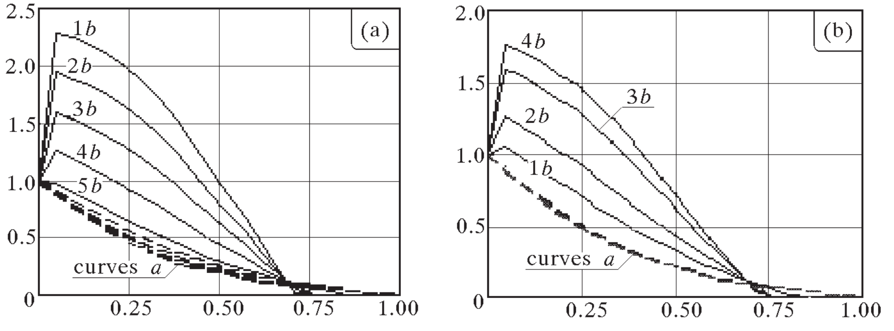

Fig. 6.

Numerical calculations show that for the case $\alpha > 1, \beta = 1$ of the sublayer beta-distribution, i.e. it is known a priori that there is the matrix near the surface $z = 0$, and sublayers position is most probable near another layer boundary $z = z_0$ (see Fig. 2), and the procedure of model homogenisation can be used effectively. We also note that for such a probable sublayer distribution, changes of the model parameters do not produce behaviour changes of the admixture concentration field. And only the change of the diffusion coefficient influences the quantitative magnitude of the admixture particles concentration in the body (Fig. 5a).

An altogether different picture emerges in the case $\alpha = 1, \beta > 1$ of the sublayer beta-distribution, i.e. the matrix is a priori on the boundary $z = z_0$ and sublayers position is the most probable near the boundary $z = 0$ (Fig. 2). In this case, using of the homogenisation procedure is inefficient. Change of the model parameters can essentially affect the behaviour of the concentration field. Thus, for example, if the diffusion coefficient of the matrix is larger than one in the sublayer material then increase of the admixture particles concentration occurs near the surface $z = 0$. And when the matrix diffusion coefficient is less than one in sublayers, accumulation of the admixture particles concentration occurs near another layer boundary $z = z_0$ (Fig. 5a). The value of the sublayer volume fraction (Fig. 6a) and its thickness (Fig. 6b) affect essentially the concentration values, without changing the function behaviour.

Remark that the obtained expressions for the admixture concentration field averaged over the ensemble of phase configurations give the possibility to determine also the dispersion of the concentration field by using the known formula (Rytov et al., 1978). It is important, in particular, to verify the obtained values of the averaged concentration.

So we can obtain the practically important information on the character of the admixture distribution in a body using some a priori data concerning their structure and physical properties.

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Dyfuzja substancji domieszkowej w dwufazowej warstwie losowo niejednorodnej

Rozważona jest jednowymiarowa (pionowa) dyfuzja substancji domieszkowej w warstwie tworzonej przez losowo-niejednorodny, dwufazowy materiał warstwowy. Przy konstruowaniu rozwiazań uwzględniono zarówno różnice współczynników dyfuzji i gęstości w różnych fazach, jak i nieciągłości współczynnika dyfuzji na granicach faz. Zgodnie z zaproponowanym podejściem przy rozwiązaniu zagadnienia brzegowego dyfuzji wpływ niejednorodności materiału sprowadzą się do rozpatrywania źródeł wewnętrznych masy, a same zagadnienie – do równania całkowego, które z kolei rozwiązano metodą rozwinięcia w szereg Neymana. Uśrednienie przybliżonego rozwiązania po zbiorze konfiguracji faz, z których złożone jest ciało, wykonano dla równomiernego losowego rozkładu faz oraz dwóch szczegółowych przypadków rozkładu beta. Porównanie rozkładów uśrednionego pola koncentracji i koncentracji w jednorodnym ośrodku pokazało potrzebę wzięcia pod uwagę zarówno różnych dyfuzyjnych właściwości faz, jak i nieciągłości współczynnika dyfuzji na granicach faz w warunkach doskonałego kontaktu. Oprócz wyznaczono zależność uśrednionej koncentracji składnika domieszkowego od współczynników dyfuzji, gęstości i objętościowych udziału faz dla losowego rozkładu beta podwarstw.

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