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On diffusion processes in a two-phase random nonhomogeneous stratified semispace

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Abstract

The approach has been proposed for description of admixture diffusion in a body with a random nonhomogeneous two-phase laminar structure. Jump discontinuities of diffusion coefficient have been taken into account at interphases as well as equally probable distribution of random layers. Admixture concentration averaged over the ensemble of layer configurations, has been obtained under consideration of medium nonhomogeneties as internal sources.

Random nonhomogeneities of real media affect essentially on mass transfer processes. For accounting their influence, as a rule, it is introduced an effective diffusion coefficient [1,2]. However, it is known the cases, for example multiphase systems with substantially different diffusion coefficients in phases, when introduction and interpretation of experimental data on the basis of such effective body characteristics are nonadequate [3]. The aim of this paper is, approach preparation to description of diffusion processes in a two-phase random nonhomogeneous semispace of stratified structure taking into account discontinuous jumps of a diffusion coefficient on interphases.

Let admixture migrates in a stochastic–nonhomogeneous stratified body composed of two solid phases with different densities (see Fig. 1). Diffusion coefficients can differ essentially in these phases. We assume that each phase is distributed by equally probable distribution in the body region. Let region $V_i^{(j)}$ takes up i-layer of j-phase, i is a layer number, $i = \overline{1, n_j}$, n_j is a number of j-kind layers.

For corresponding volumes we have

$$\bigcup_{i=1}^{n_j} V_i^{(j)} = V_j, \quad j = 1, 2; \qquad V_1 + V_2 = V. \tag{1}$$

Here V_j is the volume which j-phase occupies; V is the body volume.

Neglecting convection component of admixture transfer, its diffusion in a random nonhomogeneous two-phase stratified semispace is written in the form [4]

$$L(z,t)c(z,t) = \rho(z)\frac{\partial c(z,t)}{\partial t} - \nabla[D(z)\nabla c(z,t)] = 0, \tag{2}$$

where $c(z,t)$ denotes admixture concentration in the body, $\rho(z)$ a random body density and $D(z)$ is a random diffusion coefficient, $\nabla = \partial/\partial z$. Let's assume that body density and diffusion coefficient are constant in the volume of each phase.

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

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

and initial and boundary conditions are also given

$$c(z,t)|_{z\to\infty} = 0, \quad c(z,t)|_{t=0} = 0. \tag{3}$$

Let's introduce into consideration random operator that can be represented by unit step function

$$\eta_{ij}(z) = \begin{cases} 1, & z \in V_i^{(j)}, \\ 0, & z \notin V_i^{(j)}. \end{cases} \tag{4}$$

Then coefficients $D(z)$ and $\rho(z)$ in Eq. (2) are presented by the random operator (4) as follows

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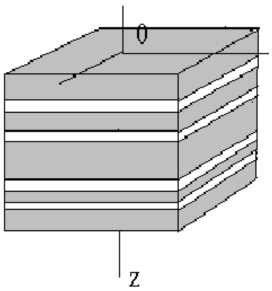

Fig. 1. One of possible realizations of a body structure.

$$D(z)=\sum_{j=1}^{2}\sum_{i=1}^{n_j}D_j\eta_{ij}(z),\qquad \rho(z)=\sum_{j=1}^{2}\sum_{i=1}^{n_j}\rho_j\eta_{ij}(z),\tag{5}$$

where D_j, ρ_j denote values of respective coefficients in the j-phase. Let's notice that

$$\sum_{j=1}^{2}\sum_{i=1}^{n_j}\eta_{ij}(z)=1.\tag{6}$$

Relationship (6) imports body continuity. Substitute coefficient representation (5) into Eq. (1) and allow for that on interphases [4]

$$\sum_{j=1}^{2}\sum_{i=1}^{n_j}\nabla\left(D_j\eta_{ij}(z)\right)=\sum_{j=1}^{2}\sum_{i=1}^{n_j}\left[D_j\right]_\Gamma\delta\left(z-z_{ij}^{\Gamma}\right),\tag{7}$$

where $[D_j]_\Gamma$ denotes a jump of diffusion coefficient on boundaries of the i-layer of j-phase ($V_i^{(j)}$), $\delta(z)$ is Dirac delta-function, z_{ij}^{Γ} is a boundary of subregion $V_i^{(j)}$.

Then we obtain

$$L(z,t)c(z,t)=\sum_{j=1}^{2}\sum_{i=1}^{n_j}L_{ij}(z,t)c(z,t)=0,\tag{8}$$

where random operator L_{ij} is

$$L_{ij}(z,t)=\rho_j\eta_{ij}(z)\frac{\partial}{\partial t}-D_j\eta_{ij}(z)\frac{\partial^2}{\partial z^2}-\big[[D_j]_\Gamma\delta(z-z_{ij}) - [D_j]_\Gamma\delta\big(z-(z_{ij}+\delta z_j)\big)\big]\frac{\partial}{\partial z}.\tag{9}$$

Here z_{ij} denotes the high boundary of the layer $V_i^{(j)}$ (random variable); δz_j is a characteristic (mean) width of the j-phase layer.

Add and subtract deterministic operator $L_m(z,t)$ defined at all interval ($t\in[0;\infty[,\ z\in[0;\infty[$):

$$L_m(z,t)=\rho_m\frac{\partial}{\partial t}-D_m\frac{\partial^2}{\partial z^2},\tag{10}$$

which coefficients are $\rho_m=\sum_{j=1}^{2}v_j\rho_j$, $D_m=\sum_{j=1}^{2}v_jD_j$ and v_j is a volume fraction of the j-phase. Then allowing for condition (6) we have

$$L_m(z,t)c(z,t)=L_{ij}^m(z,t)c(z,t),\tag{11}$$

where

$$L_{ij}^m(z,t)\equiv L_m-L=\sum_{j=1}^{2}\left(\rho_m-\rho_j\right)\sum_{i=1}^{n_j}\eta_{ij}(z)\frac{\partial}{\partial t} -\sum_{j=1}^{2}\left(D_m-D_j\right)\sum_{i=1}^{n_j}\eta_{ij}(z)\frac{\partial^2}{\partial z^2} -\sum_{j=1}^{2}\sum_{i=1}^{n_j}\big[\left(D_j-D_{j-1}\right)\delta(z-z_{ij}) + \left(D_{j+1}-D_j\right)\delta\big(z-(z_{ij}+\delta z_j)\big)\big]\frac{\partial}{\partial z}.\tag{12}$$

We consider the right-hand side of Eq. (11) as a source, i.e., medium nonhomogeneity is treated as internal sources. The solution of initial-boundary value problem (11), (3) is found in the form of Neyman series. Let $c_m(z,t)$ is a deterministic function of admixture concentration in the body with characteristics ρ_m, D_m. It satisfies following homogeneous equation

$$L_m(z,t)c_m(z,t)=0,\tag{13}$$

and initial-boundary conditions (3), i.e., [5,6]

$$c_m(z,t)=c^*\mathrm{erfc}\left\{\frac{\sqrt{\rho_m}z}{2\sqrt{D_mt}}\right\}.\tag{14}$$

Write $G(z,z')$ for unperturbed Green function satisfying a diffusion equation for point source

$$\rho_m\frac{\partial G(z,z')}{\partial t}-D_m\frac{\partial^2G(z,z')}{\partial z^2}=\delta(z-z'),\tag{15}$$

and initial and boundary conditions

$$G(z,z')\big|_{t=0}=0,\qquad G(z,z')\big|_{z=0}=G(z,z')\big|_{z\to\infty}=0.\tag{16}$$

Using (11) we obtain the following integral equation for random function of concentration $c(z,t)$ in the two-phase stratified semispace

$$c(z,t)=c_m(z,t)+\int_0^\infty G(z,z')L_{ij}^m(z',t)c(z',t)\,\mathrm{d}z'.\tag{17}$$

Neyman series for the problem (11), (3) is built by iterating the integral equation (17)

$$c(z,t)=c_m(z,t)+\int_0^\infty G(z,z')L_{ij}^m(z',t)c_m(z',t)\,\mathrm{d}z' +\int_0^\infty\int_0^\infty G(z,z')L_{ij}^m(z',t)G(z',z'') \times L_{ij}^m(z'',t)c_m(z'',t)\,\mathrm{d}z'\,\mathrm{d}z''+\dots\tag{18}$$

The first term of Neyman series (18) is the admixture concentration $c_m(z,t)$ in the homogeneous medium with physical characteristics ρ_m, d_m . The second summand

$$c^1(z,t) = \int_0^\infty G(z,z')L_{ij}^m(z',t)c_m(z',t)\,\mathrm{d}z', \tag{19}$$

describes disturbances of the concentration field which arise at the expense of availability of layers with other physical characteristics in the body. In other words, allowing for the form of the operator $L_{ij}^m(z,t)$ (12) we can say that $c^1(z,t)$ is a sum of concentration disturbances and each of them arises when a layer with characteristics ρ_j, d_j is placed in the homogeneous medium. Remark that effects on boundaries of this layer are also taken into account. The third summand in (18) can be presented in the form similar to (19):

$$c^2(z,t) = \int_0^\infty G(z,z')L_{ij}^m(z',t)c^1(z',t)\,\mathrm{d}z'. \tag{20}$$

It complies with that disturbances which arise if two layers are placed in turn into the homogeneous medium, i.e., $c^2(z,t)$ describes effects of pair influence of such layers on the concentration field. The following summands have analogue interpretation.

The problem (15) and (16) was solved by integral transformations. As a result we have obtained

$$\begin{aligned} G(z,z') = \frac{\pi}{4D_m}\big[&\mathrm{e}^{-t}\{|z+z'| - |z-z'|\} \\ &+ (z+z')\mathrm{erf}\big(a_m(z+z')\big) \\ &- (z-z')\mathrm{erf}\big(a_m(z-z')\big)\big] \\ &+ \frac{1}{2}\sqrt{\frac{\pi t}{D_m\rho_m}}\Big[\mathrm{e}^{-b_m(z+z')^2} - \mathrm{e}^{-b_m(z-z')^2}\Big], \end{aligned} \tag{21}$$

where $a_m = \sqrt{\rho_m/(D_m t)}$ and $b_m = \rho_m/(4D_m t)$.

For finding averaged field of admixture concentration $\langle c(z,t)\rangle_{\mathrm{conf}}$, let Neyman series (18) is restricted to the first two terms:

$$c(z,t) \approx c_m(z,t) + \int_0^\infty G(z,z')L_{ij}^m(z',t)c_m(z',t)\,\mathrm{d}z'. \tag{22}$$

If we substitute operator $L_{ij}^m(z',t)$ defined by (12) into Eq. (22) we obtain

$$\begin{aligned} c(z,t) \approx c_m(z,t) &+ \int_0^\infty G(z,z')\sum_{j=1}^{2}\sum_{i=1}^{n_j}\left[(\rho_m-\rho_j)\frac{\partial c_m}{\partial t} - (D_m-D_j)\frac{\partial^2 c_m}{\partial z'^2}\right]\eta_{ij}(z')\,\mathrm{d}z' \\ &+ \int_0^\infty G(z,z')\sum_{j=1}^{2}\sum_{i=1}^{n_j}\big[(D_j-D_{j-1})\delta(z'-z_{ij}) \\ &+ (D_{j+1}-D_j)\delta\big(z'-(z_{ij}+\delta z_j)\big)\big]\frac{\partial c_m}{\partial z'}\,\mathrm{d}z'. \end{aligned} \tag{23}$$

Average random concentration field (22) over the ensemble of layer configurations with equally probable distribution. As $c_m(z,t)$ is a deterministic function then $\langle c_m(z,t)\rangle_{\mathrm{conf}} = c_m(z,t)$. Consider the first integral in (23). So long as

$$\begin{aligned} \eta_{ij}(z') &= \begin{cases} 1, & z' \in [z_{ij}; z_{ij}+\delta z_j] \\ 0, & z' \notin [z_{ij}; z_{ij}+\delta z_j] \end{cases} \\ &= \begin{cases} 1, & z'-z_{ij} \in [0;\delta z_j] \\ 0, & z'-z_{ij} \notin [0;\delta z_j] \end{cases} = \eta_{ij}(z'-z_{ij}), \end{aligned} \tag{24}$$

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

$$\langle I_1\rangle_{\mathrm{conf}} = \int_0^\infty G(z,z')\sum_{j=1}^{2}\left[(\rho_m-\rho_j)\frac{\partial c_m}{\partial t} - (D_m-D_j)\times\frac{\partial^2 c_m}{\partial z'^2}\right]\frac{1}{V}\sum_{i=1}^{n_j}\int_V \eta_{ij}(z'-z_{ij})\,\mathrm{d}z_{ij}\,\mathrm{d}z'.$$

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

$$\frac{1}{V}\sum_{i=1}^{n_j}\int_V \eta_{ij}(z'-z_{ij})\,\mathrm{d}z_{ij} = \begin{cases} v_j z'/\delta z_j, & z' < \delta z_j, \\ v_j, & z' \geqslant \delta z_j. \end{cases}$$

Then we obtain

$$\begin{aligned} \langle I_1\rangle_{\mathrm{conf}} = \sum_{j=1}^{2}\int_0^{\delta z_j} G(z,z')\Big[(\rho_m-\rho_j)\frac{\partial c_m}{\partial t} &- (D_m-D_j)\frac{\partial^2 c_m}{\partial z'^2}\Big]\frac{v_j z'}{\delta z_j}\,\mathrm{d}z' + \sum_{j=1}^{2} v_j\int_{\delta z_j}^\infty G(z,z') \\ &\times\left[(\rho_m-\rho_j)\frac{\partial c_m}{\partial t} - (D_m-D_j)\frac{\partial^2 c_m}{\partial z'^2}\right]\mathrm{d}z'. \end{aligned}$$

Consider averaging the second integral in (23). Since functions $\delta(z'-z_{ij})$ and $\delta\big(z'-(z_{ij}+\delta z_j)\big)$ depend only on a form and don't depend on medium characteristics then the correlative function equals zero. Then

$$\Big\langle [D_j]_\Gamma\,\delta(z'-z_{ij}^\Gamma)\Big\rangle_{\mathrm{conf}} = \big\langle [D_j]_\Gamma\big\rangle_{\mathrm{conf}}\Big\langle \delta(z'-z_{ij}^\Gamma)\Big\rangle_{\mathrm{conf}}. \tag{25}$$

At that

$$\big\langle [D_j]_\Gamma\big\rangle_{\mathrm{conf}} = D_m - D_j. \tag{26}$$

Averaging the second multiplier in formula (25) gives

$$\begin{aligned} \frac{1}{V}\sum_{i=1}^{n_j}\int_V \delta(z'-z_{ij})\,\mathrm{d}z_{ij} &= \frac{1}{V}\sum_{i=1}^{n_j}\int_V \delta(z'-z_{ij})\,\mathrm{d}z_{ij} \\ &= \begin{cases} v_j/\delta z_j, & z' > 0, \\ v_j/(2\delta z_j), & z' = 0. \end{cases} \end{aligned} \tag{27}$$

Averaging the second summand with δ-function is done similarly. Then allowing for (25)–(27) and definition of an improper integral we obtain

$$\langle I_2\rangle_{\mathrm{conf}} = \sum_{j=1}^{2}(D_m-D_j)\frac{v_j}{\delta z_j}\left\{-\frac{1}{2}G(z,z')\frac{\partial c_m}{\partial z'}\bigg|_{z'=\delta z_j} + \int_{+0}^{+\delta z_j} G(z,z')\frac{\partial c_m}{\partial z'}\,\mathrm{d}z'\right\}. \tag{28}$$

In consequence we obtain an expression for admixture concentration averaged over the ensemble of layers configurations in the two-phase stratified semispace

$$\langle c(z,t)\rangle_{\mathrm{conf}} = c_m(z,t) + \sum_{j=1}^{2}\frac{v_j}{\delta z_j}\int_0^{\delta z_j} G(z,z')\left[(\rho_m - \rho_j)\frac{\partial c_m}{\partial t} - (D_m - D_j)\frac{\partial^2 c_m}{\partial z'^2}\right] z'\,\mathrm{d}z' + \sum_{j=1}^{2} v_j\int_{\delta z_j}^{\infty} G(z,z')\left[(\rho_m - \rho_j)\frac{\partial c_m}{\partial t} - (D_m - D_j)\frac{\partial^2 c_m}{\partial z'^2}\right]\mathrm{d}z' + \sum_{j=1}^{2}(D_m - D_j)\frac{v_j}{\delta z_j}\left\{-\frac{1}{2}G(z,z')\frac{\partial c_m}{\partial z'}\bigg|_{z'=\delta z_j} + \int_{+0}^{+\delta z_j} G(z,z')\frac{\partial c_m}{\partial z'}\,\mathrm{d}z'\right\}. \qquad (29)$$

The averaged function of admixture concentration is obtained by substituting respective expressions for Green function (21) and admixture concentration in the homogeneous medium with average physical characteristics (14) into formula (29)

$$\begin{aligned}\frac{1}{c^*}\langle c(z,t)\rangle_{\mathrm{conf}} ={}& \mathrm{erfc}\left(\sqrt{b_m}z\right) + \sum_{j=1}^{2}\left\{\frac{\pi v_j a d_{mj}}{8\delta z_j d_m t}\mathrm{e}^{-b_m\delta z_j^2}\right.\\ &\times\left[\mathrm{e}^{-t}\left(|z+\delta z_j| - |z-\delta z_j|\right) + (z+\delta z_j)\mathrm{erf}\left(a_m(z+\delta z_j)\right)\right.\\ &- (z-\delta z_j)\mathrm{erf}\left(a_m(z-\delta z_j)\right) + \frac{2a_m}{\sqrt{\pi}}\left\{\mathrm{e}^{-b_m t(z+\delta z_j)^2}\right.\\ &\left.\left. - \mathrm{e}^{-b_m t(z+\delta z_j)^2}\right\}\right] + \frac{\pi a P_1 \mathrm{e}^{-t}}{4a_m D_m}\Big(1 - \mathrm{e}^{-b_m z^2} + \theta(z-\delta z_j)\\ &\times\left[\mathrm{e}^{-b_m z^2} - \mathrm{e}^{-b_m\delta z_j^2}\right]\Big) + \frac{\pi a \mathrm{e}^{-t}}{4D_m t}\left[B_1\mathrm{erf}(\sqrt{b_m}z)\right.\\ &\left. - B_2\mathrm{erf}(\sqrt{b_m}\delta z_1)\right] + \frac{1}{2d_m t}\sqrt{\frac{t}{b_m(1+t)}}\exp\left(-\frac{b_m t z^2}{1+t}\right)\\ &\times\left\{A_1\mathrm{erf}(x_1) - A_2\mathrm{erf}(x_2) + \sqrt{\pi}\mathrm{erf}(x_3)\right\}\\ &+ \frac{1}{2\sqrt{b_m(1+t)}}\left(\left[\frac{1}{b_m} - 1 - 3P_2\right]\mathrm{e}^{-x_1^2}\right.\\ &\left. + \left[1 - \frac{1}{b_m} - 3P_2\right]\mathrm{e}^{-x_2^2} + 4P_2\mathrm{e}^{-x_3^2}\right)\\ &\left. + \frac{\pi}{4d_m}\left[\frac{a v_j}{t^2}D_\rho\left(\frac{1}{\delta z_j}F_1 + F_2\right) + F_3\right].\right\} \qquad (30)\end{aligned}$$

Here $\theta(z)$ is Heaviside function, $d_{mj} = d_m - d_j$, $\rho_{mj} = \rho_m - \rho_j$, $a^2 = \rho_m/(\pi d_m)$,

$$A_1 = \frac{v_j D_\rho}{t(1+t)}\left\{\frac{t^2 z^2}{\delta z_j(1+t)} + \frac{\sqrt{\pi}}{2b_m}\left(\frac{1}{\delta z_j} - \frac{zt}{\sqrt{b_m(1+t)}}\right)\right\} - \frac{\sqrt{\pi}}{2}, \quad D_\rho = \rho_{mj} - \frac{\rho_m d_{mj}}{2d_m t},$$

$$A_2 = \frac{v_j D_\rho}{t(1+t)}\left\{\frac{t^2 z^2}{\delta z_j(1+t)} + \frac{\sqrt{\pi}}{2b_m}\left(\frac{1}{\delta z_j} + \frac{zt}{\sqrt{b_m(1+t)}}\right)\right\} - \frac{\sqrt{\pi}}{2}, \qquad B_1 = \frac{v_j D_\rho}{2b_m t}\theta(z-\delta z_j),$$

$$B_2 = z + \left(\frac{v_j D_\rho}{2b_m t} - z\right)\theta(z-\delta z_j),$$

$$P_1 = \frac{v_j D_\rho}{\delta z_j t} - 1, \quad P_2 = \frac{tz}{\delta z_j(1+t)},$$

$$x_1 = \delta z_j\sqrt{b_m(1+t)}(1+P_2),$$
$$x_2 = \delta z_j\sqrt{b_m(1+t)}(1-P_2), \qquad x_3 = \frac{\pi}{2}az.$$

Here we use such designation:

$$F_1 = \int_0^{\delta z_j} f(z,z',t)z'^2\mathrm{e}^{-b_m z'^2}\,\mathrm{d}z';$$
$$F_2 = \int_{\delta z_j}^{\infty} f(z,z',t)z'\mathrm{e}^{-b_m z'^2}\,\mathrm{d}z';$$

$$F_2 = \int_0^{\delta z_j} f(z,z',t)\mathrm{e}^{-b_m z'^2}\,\mathrm{d}z'$$

where $f(z,z',t) = (z+z')\mathrm{erf}(a_m(z+z')) - (z-z')\mathrm{erf}(a_m(z-z'))$.

Illustration of material nonhomogeneity influence on distribution of admixture concentration in a semispace under action of a constant source on the body boundary is presented in Figs. 2 and 3 as an example of hydrogen migration in composite Fe–Cu. The hydrogen diffusion coefficients have been taken: in iron $d_{\mathrm{Fe}} = 1.8\cdot 10^{-11}$ m^2/s, in copper $d_{\mathrm{Cu}} = 4.34\cdot 10^{-10}$ m^2/s and $\rho_{\mathrm{Fe}} = 7.8\cdot 10^3$ kg/m^2, $\rho_{\mathrm{Cu}} = 8.93\cdot 10^3$ kg/m^2 ($T = 297$ K). Full line marks, respective function for admixture concentration averaged over layer configurations calculated by (30). Dashed line identifies admixture concentration in homogeneous medium with averaged physical

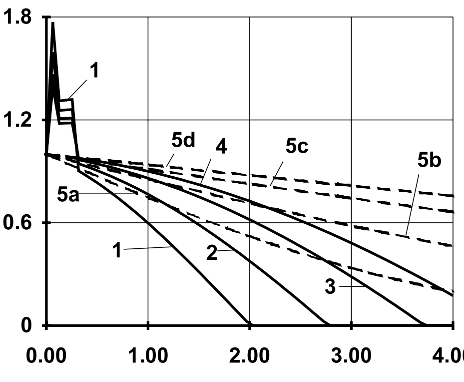

Fig. 2. Hydrogen concentration in Fe–Cu for different times.

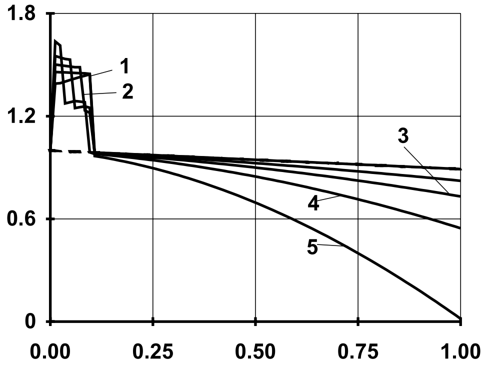

Fig. 3. Hydrogen concentration in Fe–Cu for different layer widths of copper δz_{Cu}.

characteristics. Spatial value z (m) has been laid off as abscissa, ratio of concentration H to power of constant source working on the body surface c^* has been laid off as ordinate. Distributions of concentration are compared in Fig. 2 for different moments of time at $\delta z_{\mathrm{Fe}} = 0.3$ and $\delta z_{\mathrm{Cu}} = 0.1$. Here curve 1 (5a) is presented for $t = 1.8 \cdot 10^7$ s , curve 2 (5b) shows concentration at $t = 3.15 \cdot 10^7$ s, curve 3 (5c) describes admixture concentration at $t = 5.3 \cdot 10^7$ s, and curve 4 (5d) is presented for $t = 7.45 \cdot 10^7$ s. Curves 5 describe concentrations in the homogeneous body at the same moments of time. Fig. 3 illustrates dependence of hydrogen concentration on a width of copper layers under $\delta z_{\mathrm{Fe}} = 0.1$ m at $t = 3.15 \cdot 10^7$ s . Here curve 1 shows function $c(z,t)/c^*$ under $\delta z_{\mathrm{Cu}} = 0.1$ m. Curve 2 is presented concentration H under $\delta z_{\mathrm{Cu}} = 0.07$ m. Curve 3 describes averaged concentration under $\delta z_{\mathrm{Cu}} = 0.05$ m. Curve 4 shows desired function under $\delta z_{\mathrm{Cu}} = 0.03$ m and curve 5 describes $c(z,t)/c^*$ under $\delta z_{\mathrm{Cu}} = 0.01$ m.

Numerical analysis of obtained relationships shows increase of hydrogen concentration in subsurface domain of the body with stratified Fe–Cu-structure (see 2 and 3). We suspect that body domains where it is observed increase of admixture concentration or its abrupt decrease, are brought about by availability of layers with critically greater diffusion coefficient. It is occured admixture accumulation near one boundary of a layer and abrupt fall in a vicinity of another.

Thus, for more adequate description of admixture diffusion in two-phase stratified bodies it is necessary to take into account both diffusive properties of each phase and jump discontinuities of parameters at interphase boundaries. Let's note that an effective coefficient of admixture diffusion can be introduced if the processes are considered at small time intervals (for example, $t < 10^3$–10^4 s for H transfer in Fe–Cu-structure depending on a method of effective diffusion coefficient introduction).

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