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MATHEMATICAL MODELING DIFFUSION OF DECAYING PARTICLES IN REGULAR STRUCTURES

Yevhen Chaplya[1,2] and Olha Chernukha[2]

[1]Kazimierz Wielki University in Bydgoszcz,Chodkiewicza str. 30, 85-064 Bydgoszcz, Poland
[2]Center of Mathematical Modeling of the Ukrainian National Academy of Sciences, Dudayev Str., 15, 79005 Lviv, Ukraine

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Abstract. In the paper an exact solution of the contact initial-boundary value problem is found for diffusion of decaying admixture particles in a body of a two-phase periodical stratified structure. Regularities of concentration distributions are studied to depend upon different values of a coefficient of the migrating substance's decay intensity. Conditions are established for the existence of a passage to the limit from contact initial-boundary value problems of the decaying substance diffusion to continual models of heterodiffusion by two ways allowing for the decay process. An exact solution for the partial Fisher problem for a layer is found. Mass flows are defined for the decaying admixture whose particles migrate in a horizontally regular structure.

1. INTRODUCTION

One of the current problems of today is describing and analyzing mass transfer processes in piecewise homogeneous spatially regular systems. Polycrystalline materials or fine-dispersed composite structures are often modeled by such structures. Diffusing particles in distinct domains of the system are characterized by essentially different diffusion coefficients and there is a mass exchange between domains [1-3].

Exact solutions of initial-boundary value problems of diffusion in bodies with regular structures have been formulated for a nondecaying substance in paper [4,5]. In this work, the same problem is considered for a decaying admixture. An exact solution of the corresponding contact initial-boundary value problem of diffusion is found. Mass flows in contacting domains are defined. An exact solution of the Fisher problem is also achieved by limiting the process and a set of equations of decaying particle diffusion is obtained by two ways in the continuum approximation.

2. SUBJECT OF INQUIRY AND PROBLEM FORMULATION

A body occupying a layer of thickness x_0 and composing periodically disposed domains of two types is considered. The surfaces bounding these domains are perpendicular to the layer boundaries (see Fig. 1a). Axis *Ox* is perpendicular to the body boundaries, axis *Oy* is perpendicular to the surfaces of the composing domains. Such a structure is denominated as horizontally regular or horizontally periodical. It is assumed that the domains with diffusion coefficient D_1 are $2L$ in width and the domains with coefficient D_2 are $2l$ in width. Such a structure has a family of symmetry planes ($y = \pm n(L + l)$, $n = 0,1,2\ldots$) which bisect neighbor contacting domains. Therefore, a body element can be separated on vertical boundaries of which mass fluxes equal zero in the direction parallel to the layer surfaces (in the *Oy*-axis direction, see Fig. 1b).

The $c_1(x,y,t)$ concentration of the decaying admixture in domain $\Omega_1 = [0;x_0]\times[0;L]$ is determined from the equation:

Corresponding author: Y. Chaplya, e-mail: czapla@ukw.edu.pl and O. Chernukha, e-mail: cher@cmm.lviv.ua

$$\frac{\partial c_1}{\partial t} = D_1\left[\frac{\partial^2 c_1}{\partial x^2} + \frac{\partial^2 c_1}{\partial y^2}\right] - \lambda c_1, \quad x,y \in \Omega_1. \tag{1}$$

The concentration of admixture particles $c_2(x,y,t)$ in domain $\Omega_2 =]0;x_0[\times]L;L+l]$ satisfies the following equation

$$\frac{\partial c_2}{\partial t} = D_2\left[\frac{\partial^2 c_2}{\partial x^2} + \frac{\partial^2 c_2}{\partial y^2}\right] - \lambda c_1, \quad x,y \in \Omega_2. \tag{2}$$

where λ is the coefficient of intensity of the admixture particle decay process.

We assume zero initial conditions:

$$c_1(x,y,t)\big|_{t=0} = c_2(x,y,t)\big|_{t=0} = 0. \tag{3}$$

For $t > 0$, constant values of concentrations are supported on the layer boundary $x = 0$ and they equal zero on surface $x = x_0$:

$$\begin{gathered} c_1(x,y,t)\big|_{x=0} = c_0^{(1)}, \;\; c_2(x,y,t)\big|_{x=0} = c_0^{(2)}, \\ c_1(x,y,t)\big|_{x=x_0} = c_2(x,y,t)\big|_{x=x_0} = 0 \end{gathered} \tag{4}$$

and the admixture fluxes equal zero on the lateral surfaces of the separated element $y=0$, $y=L+l$, namely:

$$\left.\frac{\partial c_1(x,y,t)}{\partial y}\right|_{y=0} = 0, \quad \left.\frac{\partial c_2(x,y,t)}{\partial y}\right|_{y=L+l} = 0. \tag{5}$$

The conditions of equalities of both the chemical potentials and the mass fluxes are imposed on the contact surface $y = L$:

$$\begin{gathered} \mu_1(x,y,t)\big|_{y=L} = \mu_2(x,y,t)\big|_{y=L}, \\ \rho_1 d_1 \left.\frac{\partial \mu_1(x,y,t)}{\partial y}\right|_{y=L} = \rho_2 d_2 \left.\frac{\partial \mu_2(x,y,t)}{\partial y}\right|_{y=L}, \end{gathered} \tag{6}$$

where $\mu_i(x,y,t)$ is the chemical potential in domain Ω_i, ρ_j is the density of domain Ω_j, d_j is a kinetic coefficient, $i = 1,2$.

Let us admit the chemical potential's linear dependence on the concentration [6]:

$$\begin{gathered} \mu_1(x,y,t) = \mu^0 - A\left(1 - \gamma_1 c_1(x,y,t)\right), \\ \mu_2(x,y,t) = \mu^0 - A\left(1 - \gamma_2 c_2(x,y,t)\right), \end{gathered}$$

where μ^0 is the chemical potential value for a clean substance in the state specified by the values of absolute temperature T and pressure P; $A=RT/M$ is a coefficient when R is an absolute gas constant

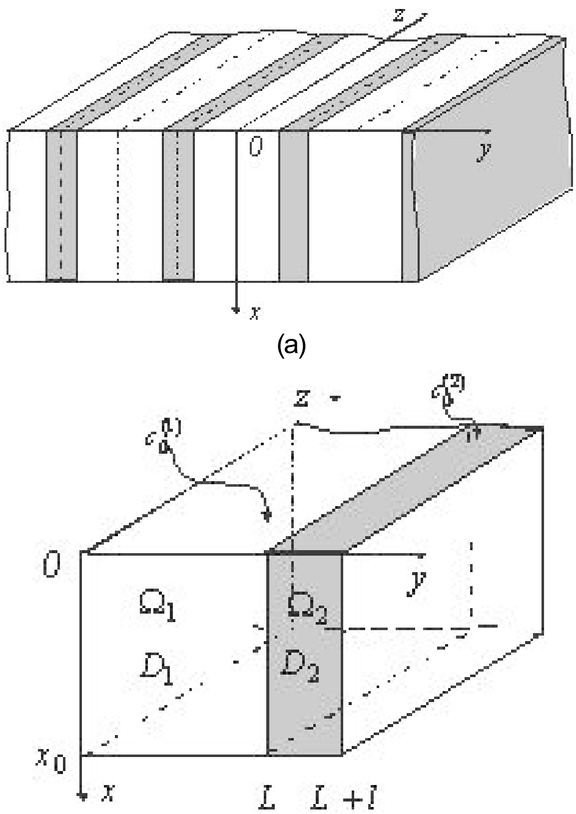


Fig. 1. A horizontally periodical body structure (a) and a separated element of the body (b).

and M is the atomic weight, γ_i is an activity factor. Then, the nonideal contact conditions for the concentrations are obtained in the form:

$$\begin{gathered} k_1 c_1(x,y,t)\big|_{y=L} = k_2 c_2(x,y,t)\big|_{y=L}, \\ \rho_1 D_1 \left.\frac{\partial c_1(x,y,t)}{\partial y}\right|_{y=L} = \rho_2 D_2 \left.\frac{\partial c_2(x,y,t)}{\partial y}\right|_{y=L}, \end{gathered} \tag{7}$$

where k_1 and k_2 are coefficients of the concentrating dependence of the chemical potentials in domains Ω_1 and Ω_2, respectively.

3. FORMULATION OF AN ANALYTICAL SOLUTION

A solution of the contact initial-boundary value problem of diffusion (1)-(5) and (7) will be found by integral transformations over space variables. We apply the finite Fourier sine transform with respect to the variable x ($x \to \alpha_n = n\pi/x_0$, $n = 1,2\ldots$; $c_i(x,y,t) \to \overline{c}_i(n,y,t)$, $i = 1,2$) [7]

$$\bar{c}_i(n,y,t) = \int_0^{x_0} c_i(x,y,t)\sin(\alpha_n x)\,\mathrm{d}x,$$

$$c_i(x,y,t) = \frac{2}{z_0}\sum_{n=1}^{\infty} \bar{c}_i(n,y,t)\sin(\alpha_n x)$$

to the problem (1)-(5) and (7). Then, it takes the form:

$$\frac{\partial \bar{c}_1}{\partial t} = D_1\frac{\partial^2 \bar{c}_1}{\partial y^2} - D_1\alpha_n^2\bar{c}_1 + D_1c_0^{(1)}\alpha_n - \lambda\bar{c}_1, \quad y\in\bar{\Omega}_1 =]0;L[; \tag{8}$$

$$\frac{\partial \bar{c}_2}{\partial t} = D_2\frac{\partial^2 \bar{c}_2}{\partial y^2} - D_2\alpha_n^2\bar{c}_2 + D_2c_0^{(2)}\alpha_n - \lambda\bar{c}_2, \quad y\in\bar{\Omega}_2 =]L;L+l[; \tag{9}$$

$$\bar{c}_1\big|_{t=0} = \bar{c}_2\big|_{t=0} = 0, \quad \frac{\partial \bar{c}_1}{\partial y}\bigg|_{y=0} = 0, \quad \frac{\partial \bar{c}_2}{\partial y}\bigg|_{y=L+l} = 0; \tag{10}$$

$$k_1\bar{c}_1\big|_{y=L} = k_2\bar{c}_2\big|_{y=L}, \quad \rho_1D_1\frac{\partial \bar{c}_1}{\partial y}\bigg|_{y=L} = \rho_2D_2\frac{\partial \bar{c}_2}{\partial y}\bigg|_{y=L}. \tag{11}$$

An integral transformation is performed with respect to the variable y separately in domains $\bar{\Omega}_1$ and $\bar{\Omega}_2$. It is necessary to know the values of the corresponding functions on boundaries of a transformation region [7] to apply the Fourier transformation. At $y = 0$ and $y = L + l$ the condition (10) defines the functions $\partial\bar{c}_1/\partial y$ on the boundary of the domain $\bar{\Omega}_1$ and $\partial\bar{c}_2/\partial y$ on the boundary of $\bar{\Omega}_2$. The values $\partial\bar{c}_i/\partial y$ are unknown on other surfaces of domains $\bar{\Omega}_1$ and $\bar{\Omega}_2$ (contact surface). They will be defined taking into account the second contact condition (11). It means that the mass fluxes on the contact boundary $y = L$ are equal and they equal the time function $g(t)$, that is:

$$\rho_1D_1\frac{\partial \bar{c}_1}{\partial y}\bigg|_{y=L} = \rho_2D_2\frac{\partial \bar{c}_2}{\partial y}\bigg|_{y=L} = g(n,L,t) \equiv g(t). \tag{12}$$

Then, the finite Fourier cosine transformation of the problem (8), (10), and (12) in the domain $\bar{\Omega}_1$ ($y \to \beta_k$; $\bar{c}_1(n,y,t) \to \tilde{c}_1(n,k,t)$) can be carried out:

$$\tilde{c}_1(n,k,t) = \int_0^{L} \bar{c}_1(n,y,t)\cos(\beta_k y)\,\mathrm{d}y, \tag{13}$$

where $\beta_k = k\pi/L$, k = 0,1,2,.... It should be noted that the Fourier sine transformation [7] is used in the contacting regions and the functions of concentration on interface considering the first contact condition are defined in the case of boundary conditions established for the sought functions.

Let us find the integral transformation from $\partial^2\bar{c}_1/\partial y^2$ first.

$$\int_0^L \frac{\partial^2\bar{c}_1}{\partial y^2}\cos(\beta_k y)\,\mathrm{d}y = \frac{\partial\bar{c}_1}{\partial y}\cos(\beta_k y)\bigg|_0^L + \beta_k\bar{c}_1\sin(\beta_k y)\big|_0^L - \beta_k^2\int_0^L \bar{c}_1\cos(\beta_k y)\,\mathrm{d}y.$$

is obtained by integrating by parts twice.

Allowing for the conditions on the boundaries of domain $\bar{\Omega}_1$ (10) and (12) we have:

$$\int_0^L \frac{\partial^2\bar{c}_1}{\partial y^2}\cos(\beta_k y)\,\mathrm{d}y = \frac{(-1)^k}{\rho_1D_1}g(t) - \beta_k^2\tilde{c}_1. \tag{14}$$

Please note that the cosine Fourier inversion in this case is [7]:

$$\bar{c}_1(n,y,t) = \frac{1}{L}\tilde{c}_1(n,0,t) + \frac{2}{L}\sum_{k=1}^{\infty}\tilde{c}_1(n,k,t)\cos(\beta_k y). \tag{15}$$

The finite Fourier cosine transformation with the account formula (14) having been applied, the initial-boundary value problem (8), (10), and (12) in the transforms is reduced to an ordinary differential equation:

$$\frac{\mathrm{d}\tilde{c}_1}{\mathrm{d}t} = -D_1\left(\alpha_n^2 + \beta_k^2 + \lambda\right)\tilde{c}_1 + D_1a_kc_0^{(1)}\alpha_n + \frac{(-1)^k}{\rho_1}g(t) \tag{16}$$

under the initial condition:

$$\tilde{c}(t)\big|_{t=0} = 0, \tag{17}$$

where $a_k = \begin{cases} L, & k = 0 \\ 0, & k = 1, 2, \ldots \end{cases}$.

A complete integral of Eq. (16) is found to read as follows [8]:

$$\tilde{c}_1(t) = e^{-\int_0^t D_1(\alpha_n^2+\beta_k^2+\lambda)dt''} \times$$
$$\left[\int_0^t \left\{ D_1 a_k c_0^{(1)} \alpha_n + \frac{(-1)^k}{\rho_1} g(t') \right\} e^{-\int_0^{t'} D_1(\alpha_n^2+\beta_k^2+\lambda)dt''} dt' + K_1 \right],$$

where K_1 is an unknown constant. As long as

$$\int_0^t D_1\left(\alpha_n^2+\beta_k^2+\lambda\right)dt' = D_1\left(\alpha_n^2+\beta_k^2+\lambda\right)t$$

$$\tilde{c}_1(t) = e^{-D_1(\alpha_n^2+\beta_k^2+\lambda)t} \times$$
$$\left[\int_0^t \left\{ D_1 a_k c_0^{(1)} \alpha_n + \frac{(-1)^k}{\rho_1} g(t') \right\} e^{-D_1(\alpha_n^2+\beta_k^2+\lambda)t'} dt' + K_1 \right],$$

Satisfying the initial condition (17) K_1=0 is obtained, and the solution of the problem (16) and (17) is:

$$\tilde{c}_1(t) = e^{-D_1(\alpha_n^2+\beta_k^2+\lambda)t} \times$$
$$\int_0^t \left[D_1 a_k c_0^{(1)} \alpha_n + \frac{(-1)^k}{\rho_1} g(t') \right] e^{-D_1(\alpha_n^2+\beta_k^2+\lambda)t'} dt'. \quad (18)$$

Let us consider the initial-boundary value problem (9), (10), and (12) in domain $\bar{\Omega}_2$. The finite Fourier cosine transformation taken over the variable y is introduced in the following way:

$$\tilde{c}_2(n,m,t) = \int_L^{L+l} \bar{c}_2(n,y,t)\cos(\beta_m(y-L))dy, \quad (19)$$

where $\beta_m = m\pi/l$. Let us search out a formula for an inverse transformation to (19). In order to do it the variable under the integral: $r = y - L$ is changed. Then, we obtain

$$\tilde{c}_2(n,m,t) = \int_0^l \bar{c}_2(n,r+L,t)\cos(\beta_m r)dr.$$

A formula of the inverse transition is known for such an integral transformation [7]:

$$\bar{c}_2(n,r+L,t) = \frac{1}{l}\tilde{c}_2(n,0,t) +$$
$$\frac{2}{l}\sum_{m=1}^{\infty}\tilde{c}_2(n,m,t)\cos(y_m r).$$

Reverting to the variable y an expression for the inverse transformation to (19) is obtained:

$$\bar{c}_2(n,y,t) = \frac{1}{l}\tilde{c}_2(n,0,t) +$$
$$\frac{2}{l}\sum_{m=1}^{\infty}\tilde{c}_2(n,m,t)\cos(\beta_m(y-L)). \quad (20)$$

Now the integral transformation (19) from $\partial^2\bar{c}_2/\partial y^2$ can be performed by analogy (14):

$$\int_L^{L+l}\frac{\partial^2\bar{c}_2}{\partial y^2}\cos(\beta_m(y-L))dy = \frac{\partial\bar{c}_2}{\partial y}\cos(\beta_m(y-L))\Big|_L^{L+l} +$$
$$\beta_m\int_L^{L+l}\frac{\partial\bar{c}_2}{\partial y}\sin(\beta_m(y-L))dy = \frac{\partial\bar{c}_2}{\partial y}\cos(\beta_m(y-L))\Big|_L^{L+l} +$$
$$\beta_m\bar{c}_2\sin(\beta_m(y-L))\Big|_L^{L+l} - \beta_m^2\int_L^{L+l}\bar{c}_m\cos(\beta_m(y-L))dy.$$

Allowing for the value $\partial\bar{c}_2/\partial y$ on the boundary of the $\bar{\Omega}_1$ and $\bar{\Omega}_2$ domain contact $y = L$ and on the lateral surface of the separated element $y = L + l$ we obtain:

$$\int_L^{L+l}\frac{\partial^2\bar{c}_2}{\partial y^2}\cos(\beta_m(y-L))dy =$$
$$\frac{(-1)^m}{\rho_2 D_2}g(t) - \beta_m^2\tilde{c}_2. \quad (21)$$

Then, the initial-boundary value problem (9), (10), and (12) takes the form:

$$\frac{d\tilde{c}_2}{dt} = -D_2\left(\alpha_n^2+\beta_m^2+\lambda\right)\tilde{c}_2 +$$
$$D_2 a_m c_0^{(2)}\alpha_n - \frac{(-1)^m}{\rho_2}g(t), \quad (22)$$

$$\tilde{c}_2(t)\big|_{t=0} = 0, \quad (23)$$

where $a_m = \begin{cases} l, & m = 0 \\ 0, & m = 1, 2, \ldots \end{cases}$. The complete integral of the ordinary differential Eq. (22) is

$$\tilde{c}_2(t) = e^{-\int_0^t D_2(\alpha_n^2+\beta_m^2+\lambda)dt''} \times$$
$$\left[\int_0^t \left\{ D_2 a_m c_0^{(2)} \alpha_n - \frac{(-1)^m}{\rho_2} g(t') \right\} e^{\int_0^{t'} D_2(\alpha_n^2+\beta_m^2+\lambda)dt''} dt' + K_2 \right],$$

here K_2 is an unknown constant. Integrating the exponents we have

$$\tilde{c}_2(t) = e^{-D_2(\alpha_n^2+\beta_m^2+\lambda)dt} \times$$
$$\left[\int_0^t \left\{ D_2 a_m c_0^{(2)} \alpha_n - \frac{(-1)^m}{\rho_2} g(t') \right\} e^{D_2(\alpha_n^2+\beta_m^2+\lambda)dt'} dt' + K_2 \right].$$

The initial condition (23) implies that $K_2 = 0$. Then, a solution of the problem (22) and (23) is obtained in the form:

$$\tilde{c}_2(t) = e^{-D_2\left(\alpha_n^2+\beta_m^2+\lambda\right)t} \times \int_0^t \left\{ D_2 a_m c_0^{(2)} \alpha_n - \frac{(-1)^m}{\rho_2} g(t') \right\} e^{D_2\left(\alpha_n^2+\beta_m^2+\lambda\right)t'} \mathrm{d}t'. \quad (24)$$

The function $g(t)$ is unknown in the expressions (18) and (24). It is obtained from the first contact condition of the concentration equality on the interface (11). In order to do it, an inverse integral cosine transformation of the concentration is performed in both the $\overline{\Omega}_1$ and $\overline{\Omega}_2$ domains by the formulae (15) and (20), respectively.

Then, taking into account the value of coefficient a_k the following formulas are obtained for function $\tilde{c}_1(n,k,t)$ in domain $\overline{\Omega}_1$:

$$\tilde{c}_1(n,0,t) = e^{-D_1\left(\alpha_n^2+\lambda\right)t} \times \int_0^t \left\{ L c_0^{(1)} \alpha_n D_1 e^{D_1\left(\alpha_n^2+\lambda\right)t'} + \frac{g(t')}{\rho_1} e^{D_1\left(\alpha_n^2+\lambda\right)t'} \right\} \mathrm{d}t',$$

$$\tilde{c}_1(n,k,t)\big|_{k\neq 0} = e^{-D_1\left(\alpha_n^2+\beta_k^2+\lambda\right)t} \frac{(-1)^k}{\rho_1} \times \int_0^t g(t') e^{D_1\left(\alpha_n^2+\beta_k^2+\lambda\right)t'} \mathrm{d}t'.$$

Using the inverse transformation formulae (15) we obtain:

$$\overline{c}_1(n,y,t) = \int_0^t \left(\left[D_1 c_0^{(1)} \alpha_n + \frac{g(t')}{L\rho_1} \right] e^{-D_1\left(\alpha_n^2+\lambda\right)(t-t')} + \frac{2}{L\rho_1} g(t') \sum_{k=1}^{\infty} (-1)^k \cos(\beta_k y) e^{-D_1\left(\alpha_n^2+\beta_k^2+\lambda\right)(t-t')} \right) \mathrm{d}t'. \quad (25)$$

Taking into account the value of coefficient a_m the following expressions for the function $\tilde{c}_2(n,m,t)$ are obtained in domain $\overline{\Omega}_2$:

$$\tilde{c}_2(n,0,t) = e^{-D_2\left(\alpha_n^2+\lambda\right)t} \times \int_0^t \left\{ l c_0^{(2)} \alpha_n D_1 e^{D_1\left(\alpha_n^2+\lambda\right)t'} - \frac{g(t')}{\rho_2} e^{D_2\left(\alpha_n^2+\lambda\right)t'} \right\} \mathrm{d}t',$$

$$\tilde{c}_2(n,m,t)\big|_{k\neq 0} = e^{-D_2\left(\alpha_n^2+\beta_m^2+\lambda\right)t} \frac{(-1)^{m+1}}{\rho_1} \times \int_0^t g(t') e^{D_2\left(\alpha_n^2+\beta_m^2+\lambda\right)t'} \mathrm{d}t'.$$

Then, the original cosine transformation with a shift of the function $\tilde{c}_2(n,m,t)$ is obtained in the form:

$$\overline{c}_2(n,y,t) = \int_0^t \left(\left[D_2 c_0^{(2)} \alpha_n + \frac{g(t')}{l\rho_2} \right] e^{-D_2\left(\alpha_n^2+\lambda\right)(t-t')} - \frac{2}{L\rho_2} g(t') \sum_{k=1}^{\infty} (-1)^m \cos(\beta_m y) e^{-D_2\left(\alpha_n^2+\beta_m^2+\lambda\right)(t-t')} \right) \mathrm{d}t'. \quad (26)$$

The value $y = L$ is substituted in expressions (25) and (26) and equated by multiplying the functions $\overline{c}_i$ by the corresponding coefficients of the concentrating dependence of chemical potential k_i. As a result, the following equation is obtained:

$$\int_0^t \left[k_1 c_0^{(1)} \alpha_n D_1 e^{-D_1\left(\alpha_n^2+\lambda\right)(t-t')} + k_1 \frac{g(t')}{\rho_1 L} \times \left\{ e^{-D_1\left(\alpha_n^2+\lambda\right)(t-t')} + 2\sum_{k=1}^{\infty} e^{-D_1\left(\alpha_n^2+\beta_k^2+\lambda\right)(t-t')} \right\} \right] \mathrm{d}t' = \int_0^t \left[k_2 c_0^{(2)} \alpha_n D_2 e^{-D_2\left(\alpha_n^2+\lambda\right)(t-t')} - k_2 \frac{g(t')}{\rho_2 L} \times \left\{ e^{-D_2\left(\alpha_n^2+\lambda\right)(t-t')} - 2\sum_{m=1}^{\infty} e^{-D_2\left(\alpha_n^2+\beta_m^2+\lambda\right)(t-t')} \right\} \right] \mathrm{d}t', \quad (27)$$

If a definite integral of a nonperiodical function is to equal zero, it is sufficient that an integral function equals zero. Then, the equation for determining the unknown function $g(t')$ is obtained:

$$k_1 \frac{g(t')}{L\rho_1} \left\{ e^{-D_1\left(\alpha_n^2+\lambda\right)(t-t')} + 2\sum_{k=1}^{\infty} e^{-D_1\left(\alpha_n^2+\beta_k^2+\lambda\right)(t-t')} \right\} + k_2 \frac{g(t')}{l\rho_2} \left\{ e^{-D_2\left(\alpha_n^2+\lambda\right)(t-t')} + 2\sum_{m=1}^{\infty} e^{-D_2\left(\alpha_n^2+\beta_m^2+\lambda\right)(t-t')} \right\} = k_2 c_0^{(2)} \alpha_n D_2 e^{-D_2\left(\alpha_n^2+\lambda\right)(t-t')} - k_1 c_0^{(1)} \alpha_n D_1 e^{-D_1\left(\alpha_n^2+\lambda\right)(t-t')}.$$

Whence:

$$g(t') = \frac{\alpha_n \left\{ k_2 c_0^{(2)} D_2 e^{-D_2\left(\alpha_n^2+\lambda\right)(t-t')} - k_1 c_0^{(1)} D_1 e^{-D_1\left(\alpha_n^2+\lambda\right)(t-t')} \right\}}{\frac{k_1}{L\rho_1} e^{-D_1\left(\alpha_n^2+\lambda\right)(t-t')} + \frac{k_2}{l\rho_2} e^{-D_2\left(\alpha_n^2+\lambda\right)(t-t')} + 2S_n(t-t')}, \quad (28)$$

where

$$S_n(t-t') = \sum_{j=1}^{\infty} \left[\frac{k_1}{L\rho_1} e^{-D_1\left(\alpha_n^2+\lambda+(j\pi/L)^2\right)(t-t')} + \frac{(-1)^j k_2}{l\rho_2} e^{-D_2\left(\alpha_n^2+\lambda+(j\pi/l)^2\right)(t-t')} \right].$$

It should be noted that the integral Eq. (27) has a non-unique solution because there exist such functions $F(t') \neq 0$ that $\int_0^t F(t')\,\mathrm{d}t' = 0$. At the same time, the original problem solution is unique independently of the chosen manner of solving the integral equation, since the function $g(t')$ in the solutions c_1 and c_2 appears only under the integral of variable t'.

The only thing remaining to obtain a final solution of the contact initial-boundary value problem (1)-(5) and (7) is to make the inverse Fourier sine transformation of the expressions (25) and (26). Then, we find:

$$c_1(x,y,t) = c_0^{(1)}\left(1 - \frac{x}{x_0}\right) - \frac{2}{x_0}\sum_{n=1}^{\infty} e^{-D_1\left(\alpha_n^2+\lambda\right)t} \times \sin(\alpha_n x)\left\{\frac{c_0^{(1)}}{\alpha_n}D_1 - \frac{1}{\rho_1 L}\int_0^t g(t')e^{D_1\left(\alpha_n^2+\lambda\right)t'}\,\mathrm{d}t' + \frac{2}{\rho_1 L}\sum_{k=1}^{\infty}(-1)^k e^{-D_1\beta_k^2 t}\cos(\beta_k y) \times \int_0^t g(t')e^{D_1\left(\alpha_n^2+\beta_k^2+\lambda\right)t'}\,\mathrm{d}t'\right\}, \tag{29}$$

$$c_2(x,y,t) = c_0^{(2)}\left(1 - \frac{x}{x_0}\right) - \frac{2}{x_0}\sum_{n=1}^{\infty} e^{-D_2\left(\alpha_n^2+\lambda\right)t} \times \sin(\alpha_n x)\left\{\frac{c_0^{(2)}}{\alpha_n}D_2 - \frac{1}{\rho_2 L}\int_0^t g(t')e^{D_2\left(\alpha_n^2+\lambda\right)t'}\,\mathrm{d}t' + \frac{2}{\rho_2 l}\sum_{m=1}^{\infty}(-1)^m e^{-D_2\beta_k^2 t}\cos(\beta_k y) \times \int_0^t g(t')e^{D_2\left(\alpha_n^2+\beta_k^2+\lambda\right)t'}\,\mathrm{d}t'\right\}, \tag{30}$$

where function $g(t')$ is specified by formula (28).

4. PASSAGE TO THE CONTINUUM LIMIT. DIMENSIONLESS FORM

Let us average the functions of admixture concentration $c_1(x,y,t)$ and $c_2(x,y,t)$ over the whole width of the separated body element $[0, L + l]$:

$$\breve{c}_i(x,t) = \frac{1}{L+l}\int_0^{L+l} c_i(x,y,t)\,\mathrm{d}y, \quad i = 1, 2. \tag{31}$$

Then, such averaged functions have to satisfy the following equations:

$$\frac{\partial \breve{c}_1}{\partial t} = D_1\frac{\partial^2 \breve{c}_1}{\partial x^2} - \lambda\breve{c}_1 + \frac{D_1}{L+l}\left.\frac{\partial c_1}{\partial y}\right|_{y=L},$$

$$\frac{\partial \breve{c}_2}{\partial t} = D_2\frac{\partial^2 \breve{c}_2}{\partial x^2} - \lambda\breve{c}_2 + \frac{D_2}{L+l}\left.\frac{\partial c_2}{\partial y}\right|_{y=L}.$$

If the mass fluxes on the contact boundary may be represented by such chemical potentials as:

$$\rho_1 D_1\left.\frac{\partial c_1}{\partial y}\right|_{y=L} = \theta_2\Delta\mu_2 - \theta_1\Delta\mu_1\big|_{y=L},$$

$$\rho_2 D_2\left.\frac{\partial c_2}{\partial y}\right|_{y=L} = \theta_1\Delta\mu_1 - \theta_2\Delta\mu_2\big|_{y=L},$$

θ_1, θ_2 ($\theta_1 \neq \theta_2$), here are coefficients of a correlation between fluxes and chemical potentials and $\Delta\mu_i = \mu_i - \mu^0$, the averaged functions (31) satisfy the equations:

$$\begin{aligned}
\frac{\partial \breve{c}_1}{\partial t} &= D_1\frac{\partial^2 \breve{c}_1}{\partial x^2} - \lambda\breve{c}_1 + \frac{1}{\rho_1(L+l)} \times \left(\theta_2\Delta\mu_2 - \theta_1\Delta\mu_1\right)\big|_{y=L},\\
\frac{\partial \breve{c}_2}{\partial t} &= D_2\frac{\partial^2 \breve{c}_2}{\partial x^2} - \lambda\breve{c}_2 - \frac{1}{\rho_2(L+l)} \times \left(\theta_2\Delta\mu_2 - \theta_1\Delta\mu_1\right)\big|_{y=L}.
\end{aligned} \tag{32}$$

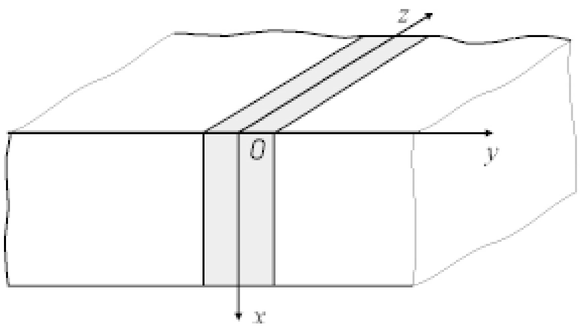
As long as $\Delta\mu_i|_{y=L} = k_i c_i|_{y=L}$, the set of equations (32) can be written in the form:

$$\frac{\partial \breve{c}_1}{\partial t} = D_1\frac{\partial^2 \breve{c}_1}{\partial x^2} - \lambda\breve{c}_1 + \frac{1}{\rho_1(L+l)} \times \left(k_2\theta_2 c_2 - k_1\theta_1 c_1\right)\big|_{y=L},$$

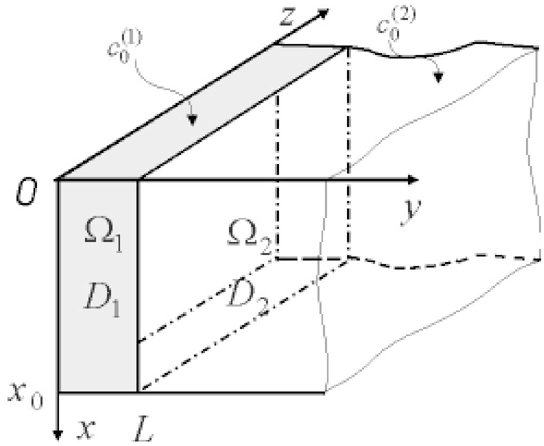
$$\frac{\partial \breve{c}_2}{\partial t} = D_2\frac{\partial^2 \breve{c}_2}{\partial x^2} - \lambda\breve{c}_2 - \frac{1}{\rho_2(L+l)} \times \left(k_2\theta_2 c_2 - k_1\theta_1 c_1\right)\big|_{y=L}.$$

If the condition $1/(L + l)c_i(x,L,t) \approx \breve{c}_i(x,t)$ takes place, we obtain a coupled set of partial differential equations of admixture heterodiffusion in two ways [9-11]:

$$\begin{aligned}
\rho_1\frac{\partial \breve{c}_1}{\partial t} &= \rho_1 D_1\frac{\partial^2 \breve{c}_1}{\partial x^2} - \lambda\breve{c}_1 - \bar{k}_1\breve{c}_1 + \bar{k}_2\breve{c}_2,\\
\rho_2\frac{\partial \breve{c}_2}{\partial t} &= \rho_2 D_2\frac{\partial^2 \breve{c}_2}{\partial x^2} - \lambda\breve{c}_2 + \bar{k}_1\breve{c}_1 - \bar{k}_2\breve{c}_2,
\end{aligned} \tag{33}$$



(a)



(b)

Fig. 2. Diffusion in a polycrystal along a grain boundary.

where $\bar{k}_1 = \theta_i k_i$ (i = 1,2) are coefficients of intensity of the particle transition process between different diffusion ways.

Thus, subject to the equality of the admixture fluxes and linear combinations of the chemical potentials on a contact boundary by means of averaging concentrations over body width, we obtain immediately a set of equations for heterodiffusion by two ways taking into account particle transitions from one migration way into another.

Now, a natural dimensionless form can be introduced for such problem [11]:

$$\tau = \bar{k}_2 t, \quad \xi = \left(\bar{k}_2 / D_1\right)^{1/2} x. \tag{34}$$

We take into consideration the dimensionless space variable $\eta = (\bar{k}_2/D_1)^{1/2}y$. The contact initial-boundary value problem (1)-(5) and (7) can be presented in the dimensionless form:

$$\frac{\partial c_1}{\partial \tau} = \frac{\partial^2 c_1}{\partial \xi^2} + \frac{\partial^2 c_1}{\partial \eta^2} - \tilde{\lambda} c_1, \qquad \xi, \eta \in \omega_1 = \left]0; \xi_0\right[\times \left]0; \Lambda\right[, \tag{35}$$

$$\frac{\partial c_2}{\partial \tau} = d\left[\frac{\partial^2 c_2}{\partial \xi^2} + \frac{\partial^2 c_2}{\partial \eta^2}\right] - \tilde{\lambda} c_2, \qquad \xi, \eta \in \omega_2 = \left]0; \xi_0\right[\times \left]\Lambda; \Lambda + \bar{\lambda}\right[; \tag{36}$$

$$c_1(\xi,\eta,\tau)\big|_{\tau=0} = c_2(\xi,\eta,\tau)\big|_{\tau=0} = 0,$$
$$c_1(\xi,\eta,\tau)\big|_{\xi=0} = c_0^{(1)}, \quad c_2(\xi,\eta,\tau)\big|_{\xi=0} = c_0^{(2)},$$
$$c_1(\xi,\eta,\tau)\big|_{\xi=\xi_0} = c_2(\xi,\eta,\tau)\big|_{\xi=\xi_0} = 0,$$

$$\left.\frac{\partial c_1(\xi,\eta,\tau)}{\partial \eta}\right|_{\eta=0} = \left.\frac{\partial c_2(\xi,\eta,\tau)}{\partial \eta}\right|_{\eta=\Lambda+\bar{\lambda}} = 0, \tag{37}$$

$$k_1 c_1\big|_{\eta=\Lambda} = k_2 c_2\big|_{\eta=\Lambda}, \quad \rho_1 \left.\frac{\partial c_1}{\partial \eta}\right|_{\eta=\Lambda} = \rho_2 d \left.\frac{\partial c_2}{\partial \eta}\right|_{\eta=\Lambda}. \tag{38}$$

Here $d = D_2/D_1$; $\tilde{\lambda} = \lambda/\bar{k}_2$, $\xi_0 = (\bar{k}_2/D_1)^{1/2}x_0$, $\Lambda = (\bar{k}_2/D_1)^{1/2}L$, $\bar{\lambda} = (\bar{k}_2/D_1)^{1/2}l$.

Thus, the proposed passage to the limit from a contact initial-boundary value problem of decaying admixture diffusion in horizontally periodical structures to continuum models of heterodiffusion by two ways gives an opportunity of not only finding solutions of heterodiffusion problems but also of using the natural dimensionless form (34) for problems of diffusion in bodies with regular structures. It should be noted that such dimensionless form does not involve any sizes of a body or its constituent regions.

5. THE FISHER PROBLEM AS A PARTICULAR CASE OF A DIFFUSION PROBLEM IN A HORIZONTALLY PERIODICAL STRUCTURE

If the domain Ω_2 width tends to infinity, $l \to \infty$ ($L \neq 0$), in the relationships (1)-(5) and (7), we obtain the Fisher problem [3,12] for a layer modeling diffusion of decaying particles in a polycrystal along a grain boundary. This is decaying admixture diffusion in a semi-infinite solid in which a thin plate has been put so that its plane should be perpendicular to the body surface (see Fig. 2). We assume that the diffuser concentration preserves its constant values on a free sample surface and the diffusion coefficient D_1 in a plate (which conforms to a grain boundary) is much greater then D_2 characterizing the mass transfer in the remaining body [3].

In the formulae (29) and (30) we pass to the limit at $l \to \infty$ and obtain the exact analytical solution of the Fisher problem for a layer:

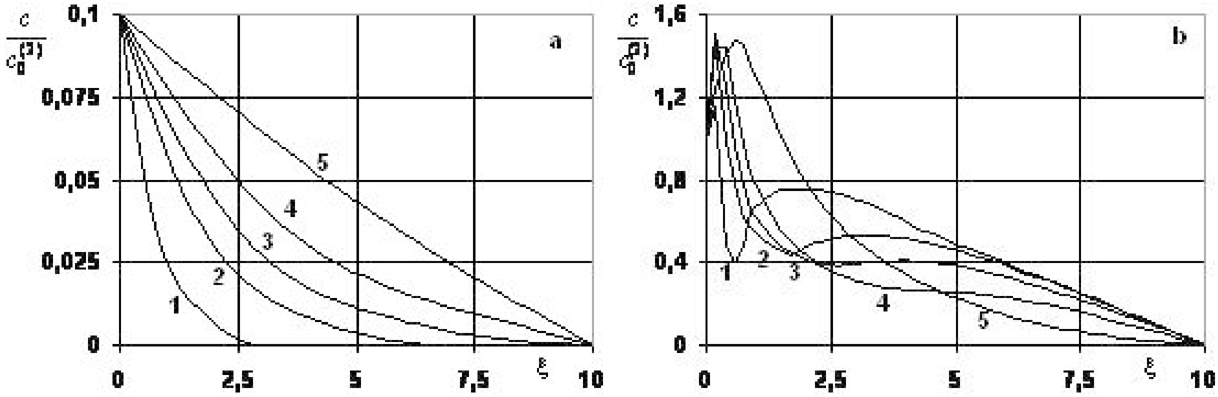


Fig. 3. Distributions of nondecaying admixture concentration along depth in different time moments at $\tilde{\lambda}$ = 0, (a) – in the middle of domain Ω_1, (b) – in the middle of domain Ω_2.

$$\lim_{l\to\infty} c_1(x,y,t) = c_0^{(1)}\left(1-\frac{x}{x_0}\right) - \frac{2}{x_0}\sum_{n=1}^{\infty}\sin(\alpha_n x)\times e^{-D_1(\alpha_n^2+\lambda)t}\left(\frac{c_0^{(1)}}{\alpha_n}D_1 - \frac{1}{L\rho_1}\int_0^t \breve{g}(t')e^{D_1(\alpha_n^2+\lambda)t'}\,\mathrm{d}t' + \frac{2}{\rho_1 L}\sum_{k=1}^{\infty}(-1)^k e^{-D_1\beta_k^2 t}\cos(\beta_k y)\times \int_0^t \breve{g}(t')e^{D_1(\alpha_n^2+\beta_k^2+\lambda)t'}\,\mathrm{d}t'\right), \quad (39)$$

$$\lim_{l\to\infty} c_2(x,y,t) = c_0^{(2)}\times \left[1-\frac{x}{x_0}-\frac{2}{x_0}\sum_{n=1}^{\infty}\frac{1}{\alpha_n}\sin(\alpha_n x)e^{-D_2(\alpha_n^2+\lambda)t}\right], \quad (40)$$

where

$$\breve{g}(t) = \frac{c_0^{(1)}D_1 L\rho_1\alpha_n}{1+2\breve{S}_n}\times \left[\frac{k_2 c_0^{(2)}D_2}{k_1 c_0^{(1)}D_1}\exp\left\{-(D_2-D_1)(\alpha_n^2+\lambda)(t-t')\right\}-1\right],$$

$$\breve{S}_n = \sum_{j=1}^{\infty} e^{-D_1\left(\lambda+(j\pi/L)^2\right)(t-t')}.$$

It should be noted that the expression (40) for decaying admixture concentration in the domain Ω_2 is identical to the solution of a one-dimensional problem of decaying particle diffusion for a layer with the diffusion coefficient D_2 and the initial and boundary conditions (3) and (4) that structurally correspond to the results mentioned in [3].

6. A NUMERICAL ANALYSIS OF THE DECAYING ADMIXTURE CONCENTRATION BEHAVIOR IN A LAYER WITH A HORIZONTALLY REGULAR STRUCTURE

An illustration of decaying admixture concentration distributions in a layer with a horizontally periodical structure computed by the formulae (29) and (30) is presented in Figs. 3-6. Numerical calculations have been conducted in the dimensionless variables τ, ξ, η introduced by (34). The problem coefficients have been taken as ξ_0 = 10; Λ = 1, $\bar{\lambda}$ = 0.1, $d = D_2/D_1$ = 0.01, ρ_2/ρ_1 = 1.5, $c_0^{(1)}/c_0^{(2)}$ = 0.1. In Figs. 3 and 4 distributions of the concentration of nondecaying ($\tilde{\lambda}$ = 0) and decaying ($\tilde{\lambda}$ = 10) admixtures along the $O\xi$-axis in different time moments τ = 1; 5; 10; 20; 100 (curves 1-5, respectively) are shown in the middle of domain Ω_1, i.e. at η = 0.5 (Fig. 3a) and at ξ = 1.05 (the middle of domain Ω_2, Fig. 3b) for $\bar{k}_1/\bar{k}_2$ = 10.

Fig. 5 illustrates the behavior of the decaying particle concentration function in dimensionless time moment τ = 10 for different values of the dimensionless coefficient of intensity of migrating substance decay $\tilde{\lambda}$ = 2, 5, 10, 20 (curves 1-4). Fig. 6 shows the decaying admixture concentration ($\tilde{\lambda}$ = 10) distributions along the $O\eta$-axis, i.e. on the width of a separated body element. Fig. 6a illustrates the dependence of function $c(\xi,\eta,\tau)/c_0^{(2)}$ on different time

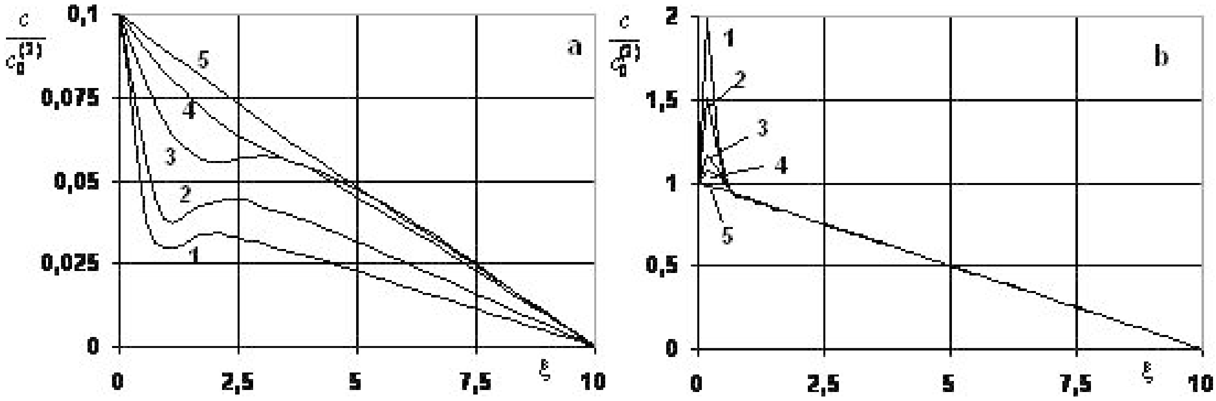


Fig. 4. Distributions of decaying admixture concentration along depth in different time moments at $\tilde{\lambda}$ = 10, (a) – in the middle of domain Ω_1, (b) – in the middle of domain Ω_2.

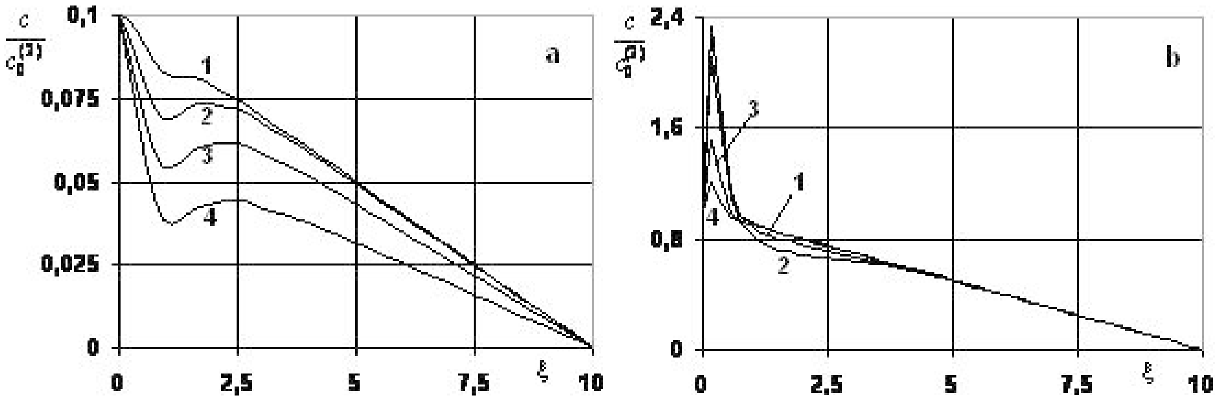


Fig. 5. Distributions of decaying admixture concentration along the body depth for different values of parameter $\tilde{\lambda}$ at τ = 10, (a) – – in the middle of domain Ω_1, (b) – in the middle of domain Ω_2.

moments τ = 1, 5, 10 (curves 1-3) at depth ξ = 1. Fig. 6b demonstrates the behavior of the concentration function depending on the diffusion coefficients ratio d = 0.1; 0.5 (curves 1 and 2). The full lines in the figure mark function $c(\xi,\eta,\tau)/c_0^{(2)}$ in moment τ = 1 and the dashed lines identify it at τ = 10.

Let us note that the admixture concentration function behavior along the layer depth is substantially different in domains Ω_1 and Ω_2 (see Figs. 3a-5a and Figs. 3b-5b) for both the decaying and nondecaying diffusing substance. Characteristic distributions of the concentration along the layer depth in case of migration of nondecaying particles in horizontally periodical structures are similar to those with a quick diffusion coefficient (see Fig. 3a) in a homogeneous layer in region Ω_1 and with a slow diffusion coefficient (see Fig. 3b) in multicomponent bodies in domain Ω_2. At the same time, if substance decay processes are taken into account, this may lead to qualitative changes in the concentration function behavior in all structural elements of the body. In particular, in case of a more active mass source on the surface, lower diffusion coefficient in domain Ω_2 and a more intensive transition of particles from Ω_2 into Ω_1, a time-decrease of the subsurface maximum of the concentration is observed in domain Ω_2 (see Fig. 4b) down to reaching the stationary regime for a homogeneous medium. Under such conditions in domain Ω_1 the subsurface local minimum being characteristic for distributions of the decaying admixture concentration (see Fig. 5a) decreases in time, the value of the concentration c_1 increases and this function reaches also the stationary regime for a homogeneous body (see Fig. 4a). A corresponding decrease in the admixture concentration values is observed for other proportions of the problem coefficients on all intervals depending on the value of the admixture particle decay coefficient.

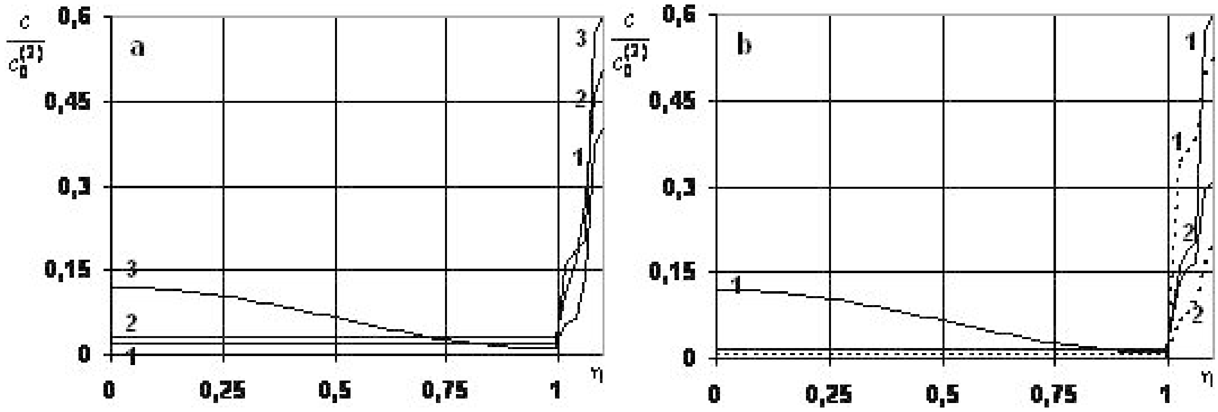


Fig. 6. Distributions of decaying admixture concentration along the body element width, (a) is shown for different time moments, (b) is shown for different values of parameter *d*.

7. MASS FLUXES OF DECAYING PARTICLES IN A LAYER WITH A HORIZONTALLY PERIODICAL STRUCTURE

The obtained analytical expressions for the decaying admixture concentrations give an opportunity to find such important characteristics of mass transfer as mass fluxes of admixture particles through any surface $x = x^*$. They are deduced by the formula:

$$J_*^{(i)}(t) = -D_i \left.\frac{\partial c_i(x,y,t)}{\partial x}\right|_{x=x^*}, \quad (x,y)\in \Omega_i,$$
$$i = 1, 2; \quad x^* \in [0; x_0]. \qquad (41)$$

Substituting the corresponding expressions for the admixture concentrations (29) and (30) into (41) we obtain the following formulae for mass fluxes through surface $x = x^*$ in domain Ω_1:

$$J_*^{(1)}(t) = \frac{D_1}{x_0}\Bigg[c_0^{(1)} + 2\sum_{n=1}^{\infty} e^{-D_1(\alpha_n^2+\lambda)t}\cos(\alpha_n x^*)\times \Bigg\{c_0^{(1)}D_1 - \frac{\alpha_n}{\rho_1 L}\int_0^t g(t')e^{D_1(\alpha_n^2+\lambda)t'}\,\mathrm{d}t' + \frac{2\alpha_n}{\rho_1 L}\sum_{k=1}^{\infty}(-1)^k e^{-D_1\beta_k^2 t}\cos(\beta_k y)\times \int_0^t g(t')e^{D_1(\alpha_n^2+\beta_k^2+\lambda)t'}\,\mathrm{d}t'\Bigg\}\Bigg], \qquad (42)$$

in domain Ω_2:

$$J_*^{(2)}(t) = \frac{D_2}{x_0}\Bigg[c_0^{(2)} + 2\sum_{n=1}^{\infty} e^{-D_1(\alpha_n^2+\lambda)t}\cos(\alpha_n x^*)\times \Bigg\{c_0^{(2)}D_2 - \frac{\alpha_n}{\rho_2 l}\int_0^t g(t')e^{D_1(\alpha_n^2+\lambda)t'}\,\mathrm{d}t' + \frac{2\alpha_n}{\rho_2 l}\sum_{m=1}^{\infty}(-1)^m e^{-D_1\beta_m^2 t}\cos(\beta_m y)\times \int_0^t g(t')e^{D_2(\alpha_n^2+\beta_m^2+\lambda)t'}\,\mathrm{d}t'\Bigg\}\Bigg]. \qquad (43)$$

In particular, mass fluxes through the layer surface $x=x_0$ ($x^*=x_0$) take the form:
in domain Ω_1:

$$J_0^{(1)}(t) = \frac{D_1}{x_0}\Bigg[c_0^{(1)} + 2\sum_{n=1}^{\infty}(-1)^n e^{-D_1(\alpha_n^2+\lambda)t}\times \Bigg\{c_0^{(1)}D_1 - \frac{\alpha_n}{\rho_1 L}\int_0^t g(t')e^{D_1(\alpha_n^2+\lambda)t'}\,\mathrm{d}t' + \frac{2}{\rho_1 L}\sum_{k=1}^{\infty}(-1)^k e^{-D_1\beta_k^2 t}\cos(\beta_k y)\times \int_0^t g(t')e^{D_1(\alpha_n^2+\beta_k^2+\lambda)t'}\,\mathrm{d}t'\Bigg\}\Bigg],$$

in domain Ω_2:

$$J_*^{(2)}(t) = \frac{D_2}{x_0}\left[c_0^{(2)} + 2\sum_{n=1}^{\infty}(-1)^n e^{-D_1\left(\alpha_n^2+\lambda\right)t} \times \right.$$
$$\left\{c_0^{(2)} D_2 - \frac{\alpha_n}{\rho_2 l}\int_0^t g(t')e^{D_1\left(\alpha_n^2+\lambda\right)t'}\,\mathrm{d}t' + \right.$$
$$\frac{2}{\rho_2 l}\sum_{m=1}^{\infty}(-1)^m e^{-D_1\beta_m^2 t}\cos\left(\beta_m y\right)\times$$
$$\left.\left.\int_0^t g(t')e^{D_2\left(\alpha_n^2+\beta_m^2+\lambda\right)t'}\,\mathrm{d}t'\right\}\right].$$

In the same way mass fluxes of decaying particles through any vertical surface $y=y^*$can be found.

8. CONCLUSION

In this work we have considered formulating an analytical solution of the contact initial-boundary value problem of decaying admixture diffusion in horizontally periodical structures. The method is based on application of integral transformations over space variables separately in contacting domains. Finding such analytical expressions for the decaying admixture concentration gives an opportunity to define total mass fluxes through any body surface. Obtaining the exact solution of such problem makes it also possible to find exact solutions for particular practically important initial-boundary value problems (e.g. the Fisher problem).

The conditions have been determined, under which a relation between a problem of decaying particle diffusion in a body with a horizontally periodical structure and a problem of one-dimensional heterodiffusion by two ways, have been established. It gives a possibility to introduce a natural dimensionless form for a problem of mass transfer in horizontally regular structures, too.

It should be noted that no conditions on the sizes of contacting domains are used in the proposed method for formulating an exact solution of the contact initial-boundary value problems. Hence, it can be suitable both for bodies with comparable sizes of contacting regions and in cases when one domain width is much greater (or smaller) than the other.

And finally, it should be noted that when considering the form of Eqs. (1) and (2) the solutions of problems of mass transfer in horizontally regular structures can be applied for studying heat transfer processes in such bodies by treating the ideal contact conditions as a partial case of the one presented in this work.

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