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International Journal of Heat and Mass Transfer 48 (2005) 2290–2298
International Journal of HEAT and MASS TRANSFER
www.elsevier.com/locate/ijhmt

Admixture mass transfer in a body with horizontally periodical structure

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Received 17 September 2004
Available online 17 March 2005

Abstract

Admixture mass transfer is studied in geometrically complex systems. The method is proposed for finding an exact solution of initial-boundary value problem of diffusion in bodies with two-phase periodical structure. It is based on application of integral transformations with respect to space variables in contacting areas. The behaviour of mass transfer processes in such systems is investigated. The relation between problems of mass transfer in horizontally periodical structure and heterodiffusion by two ways is found.

Keywords: Admixture diffusion; Periodical structure; Initial-boundary value problem; Contact conditions; Integral transformation

1. Introduction

The problem of describing and analyzing diffusion process in bodies with complex internal structure arises frequently at solving practical tasks. When body material is fine-dispersed and we can assume that in every arbitrarily chosen small body region there are always its all structural elements then we can use continual approaches of rational mechanics [1] or nonequilibrium thermodynamics [2] for describing processes of admixture transport. With that we regard that particles of the same chemical kind occur locally in physically different states distinguishing, in particular, by their diffusion coefficients. Then admixture transport comes about by several ways (their number corresponds quantity of physically different states). And it is accompanied by particles intertransitions from one migration way into the others.

At the same time exact solutions of concrete contact initial-boundary value problems of transfer processes for sectionally homogeneous (in particular, space regular) systems [3] are of interest. Such medium can consists of contacting homogeneous subsystems, which exchange by substance. Regular structures, which elements have different diffusive properties, are considered at investigation of mass transfer in polycrystals along grain boundaries and dislocations [4,5] or in porous media, for example soils, consisting from monocrystals and canals of particles quick transport [6–8].

Notice that finding analytical solutions of contact initial-boundary value problems on basis of classical methods of mathematical physics gives rise to some difficulties. So it is proposed an original method for constructing exact solutions of initial-boundary value problems of diffusion in bodies with regular structure on basis of application of integral transformations. Exact

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0017-9310/$ - see front matter
doi:10.1016/j.ijheatmasstransfer.2005.01.003

analytical solutions of such problems give an opportunity to analyze bound of applicability of known solutions of the problems in bodies with a solitary inclusion [4,5] and to perform boundary transitions to continual models of heterodiffusion by way for estimation of diffusion coefficients.

2. Subject of inquiry and problem formulation

Consider a body occupying a layer of thickness x_0 and composing periodically disposed areas of two types. Surfaces bounded these areas are perpendicular to the layer boundaries (see Fig. 1a). Axis Ox is perpendicular to body boundaries, Oy is perpendicular to surfaces of composing areas. We denominate such structure as horizontally regular or horizontally periodical one. Assume that areas with diffusion coefficient D_1 have width $2L$ and width of areas with coefficient D_2 is $2l$. Such structure has a family of symmetry planes ($y = \pm n(L + l)$, $n = 0, 1, 2, \ldots$) which bisect neighbour contacting areas. Therefore we can separate out a body element, on vertical boundaries of which mass fluxes equal zero in the direction being parallel to the layer surfaces (in the direction Oy-axis, see Fig. 1b).

Admixture concentration $c_1(x, y, t)$ in the area $\Omega_1 =]0; x_0[\times]0; L[$ is determined from the equation

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

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

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

Assume zero initial conditions

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

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

$$c_1(x, y, t)|_{x=0} = c_0^{(1)} \equiv \text{constant},$$
$$c_2(x, y, t)|_{x=0} = c_0^{(2)} \equiv \text{constant};$$

$$c_1(x, y, t)|_{x=x_0} = c_2(x, y, t)|_{x=x_0} = 0, \tag{4}$$

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

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

On the contact surface $y = L$ we impose conditions of equalities of both chemical potentials and mass fluxes:

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

where $\mu_i(x, y, t)$ is a chemical potential in area Ω_i, ρ_i is a density of area Ω_i, d_i is a kinetic coefficient, $i = 1, 2$.

Let admit linear dependence of chemical potential on concentration [9]

$$\mu_1(x, y, t) = \mu^0 - A(1 - \gamma_1 c_1(x, y, t)),$$
$$\mu_2(x, y, t) = \mu^0 - A(1 - \gamma_2 c_2(x, y, t)),$$

where μ^0 is a chemical potential value for clean substance in the state specified by values of absolute temperature T and pressure P; $A = RT/M$ is a coefficient when R is absolute gas constant and M is an atomic weight, γ_i is an activity factor. Then we obtain the conditions of nonideal contact for concentrations in the form

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

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

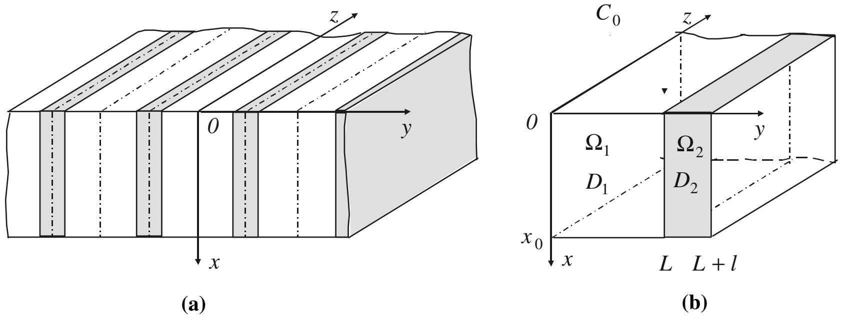

Fig. 1. Horizontally periodical body structure (a) and separated element of the body (b).

3. Construction of analytical solution

Find the solution of contact initial-boundary value problem of diffusion (1)–(5) and (7) by integral transformations over space variables. Apply finite Fourier sine transform with respect to variable x ($x \to x_n = n\pi/x_0$, $n = 1,2,\ldots$; $c_i(x,y,t) \to \bar{c}_i(n,y,t)$, $i = 1,2$) [10]

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

$$c_i(x,y,t) = \frac{2}{x_0}\sum_{n=1}^{\infty}\bar{c}_i(n,y,t)\sin(x_n x)$$

to the problem (1)–(5) and (7). Then it takes the form

$$\frac{\partial\bar{c}_1}{\partial t} = D_1\frac{\partial^2\bar{c}_1}{\partial y^2} - D_1 x_n^2\bar{c}_1 + D_1 c_0^{(1)}x_n, \quad y \in \overline{\Omega}_1 =]0;L[; \tag{8}$$

$$\frac{\partial\bar{c}_2}{\partial t} = D_2\frac{\partial^2\bar{c}_2}{\partial y^2} - D_2 x_n^2\bar{c}_2 + D_2 c_0^{(2)}x_n, \quad y \in \overline{\Omega}_2 =]L;L+l[; \tag{9}$$

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

$$k_1\bar{c}_1|_{y=L} = k_2\bar{c}_2|_{y=L}, \quad \rho_1 D_1\left.\frac{\partial\bar{c}_1}{\partial y}\right|_{y=L} = \rho_2 D_2\left.\frac{\partial\bar{c}_2}{\partial y}\right|_{y=L}. \tag{11}$$

Perform an integral transformation with respect to variable y apart in area $\overline{\Omega}_1$ and $\overline{\Omega}_2$. For applying Fourier transformation it is necessary to know values of corresponding functions on boundaries of a transformation region [10]. At $y = 0$ and $y = L + l$ the condition (10) defines functions $\partial\bar{c}_1/\partial y$ on the boundary of area $\overline{\Omega}_1$ and $\partial\bar{c}_2/\partial y$ on the boundary $\overline{\Omega}_2$. Values $\partial\bar{c}_i/\partial y$ are unknown on another surfaces of areas $\overline{\Omega}_1$ and $\overline{\Omega}_2$ (contact surface). Define them taking into account the second contact condition (11). It means that mass fluxes are equal on the contact boundary $y = L$ and they equal some time function $g(t)$, i.e.

$$\rho_1 D_1\left.\frac{\partial\bar{c}_1}{\partial y}\right|_{y=L} = \rho_2 D_2\left.\frac{\partial\bar{c}_2}{\partial y}\right|_{y=L} = g(n,L,t) \equiv g(t). \tag{12}$$

Then we can carry out finite Fourier cosine transformation of the problem (8), (10) and (12) in the area $\overline{\Omega}_1$ ($y \to y_k$; $\bar{c}_1(n,y,t) \to \tilde{c}_1(n,k,t)$):

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

where $y_k = k\pi/L$, $k = 0,1,2,\ldots$. Notice that in the case of boundary conditions established for sought functions we use Fourier sine transformation [10] in contacting regions and define functions of concentration on interface considering the first contact condition.

Find integral transformation from $\partial^2\bar{c}_1/\partial y^2$ first. Twice integrating by parts we obtain

$$\int_0^L \frac{\partial^2\bar{c}_1}{\partial y^2}\cos(y_k y)\,dy = \left.\frac{\partial\bar{c}_1}{\partial y}\cos(y_k y)\right|_0^L + y_k\bar{c}_1\sin(y_k y)|_0^L - y_k^2\int_0^L \bar{c}_1\cos(y_k y)\,dy.$$

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

$$\int_0^L \frac{\partial^2\bar{c}_1}{\partial y^2}\cos(y_k y)\,dy = \frac{(-1)^k}{\rho_1 D_1}g(t) - y_k^2\tilde{c}_1. \tag{14}$$

Remark that in this case cosine Fourier inversion is [10]

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

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

$$\frac{d\tilde{c}_1}{dt} = -D_1(x_n^2 + y_k^2)\tilde{c}_1 + D_1 a_k c_0^{(1)}x_n + \frac{(-1)^k}{\rho_1}g(t) \tag{16}$$

under initial condition

$$\tilde{c}_1(t)|_{t=0} = 0, \tag{17}$$

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

We find a complete integral of Eq. (16) as follows [11]:

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

where K_1 is an unknown constant. So long as $\int_0^t D_1(x_n^2 + y_k^2)\,dt' = D_1(x_n^2 + y_k^2)t$ then

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

Satisfying initial condition (17) we obtain $K_1 = 0$. And the solution of problem (16) and (17) is

$$\tilde{c}_1(t) = e^{-D_1(x_n^2+y_k^2)t}\int_0^t\left[D_1 a_k c_0^{(1)}x_n + \frac{(-1)^k}{\rho_1}g(t')\right]e^{D_1(x_n^2+y_k^2)t'}\,dt'. \tag{18}$$

Let us consider initial-boundary value problem (9), (10) and (12) in the area $\overline{\Omega}_2$. Introduce finite Fourier cosine transformation taken over variable y like that

$$\tilde{c}_2(n,m,t) = \int_L^{L+l} \bar{c}_2(n,y,t)\cos(y_m(y-L))\,\mathrm{d}y, \qquad (19)$$

where $y_m = m\pi/l$. Search out a formular for inverse transformation to (19). In order to do it we change variable under the integral: $r = y - L$. Then we obtain

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

For such integral transformation a formula of inverse transition is known [10]:

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

Reventing to the variable y we obtain an expression for inverse transformation to (19)

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

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

$$\begin{aligned}\int_L^{L+l}&\frac{\partial^2\bar{c}_2}{\partial y^2}\cos(y_m(y-L))\,\mathrm{d}y\\ &= \frac{\partial\bar{c}_2}{\partial y}\cos(y_m(y-L))\Big|_L^{L+l} + y_m\int_L^{L+l}\frac{\partial\bar{c}_2}{\partial y}\sin(y_m(y-L))\,\mathrm{d}y\\ &= \frac{\partial\bar{c}_2}{\partial y}\cos(y_m(y-L))\Big|_L^{L+l} + y_m\bar{c}_2\sin(y_m(y-L))|_L^{L+l}\\ &\quad - y_m^2\int_L^{L+l}\bar{c}_m\cos(y_m(y-L))\,\mathrm{d}y.\end{aligned}$$

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

$$\int_L^{L+l}\frac{\partial^2\bar{c}_2}{\partial y^2}\cos(y_m(y-L))\,\mathrm{d}y = \frac{(-1)^m}{\rho_2 D_2}g(t) - y_m^2\tilde{c}_2. \qquad (21)$$

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

$$\frac{\mathrm{d}\tilde{c}_2}{\mathrm{d}t} = -D_2(x_n^2+y_m^2)\tilde{c}_2 + D_2 a_m c_0^{(2)}x_n - \frac{(-1)^m}{\rho_2}g(t), \qquad (22)$$

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

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

$$\tilde{c}_2(t) = \mathrm{e}^{-\int_0^t D_2(x_n^2+y_k^2)\mathrm{d}t''}\left[\int_0^t\left\{a_m c_0^{(2)}x_n D_2 + \frac{(-1)^{m+1}}{\rho_2}g(t')\right\}\mathrm{e}^{-\int_0^{t'} D_2(x_n^2+y_k^2)\mathrm{d}t''}\,\mathrm{d}t' + K_2\right],$$

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

$$\tilde{c}_2(t) = \mathrm{e}^{-D_2(x_n^2+y_m^2)t}\left[\int_0^t\left\{D_2 a_m c_0^{(2)}x_n - \frac{(-1)^m}{\rho_2}g(t')\right\}\mathrm{e}^{D_2(x_n^2+y_m^2)t'}\,\mathrm{d}t' + K_2\right].$$

The initial condition (23) implies that $K_2 = 0$. Then we obtain the solution of problem (22) and (23) in the form

$$\tilde{c}_2(t) = \mathrm{e}^{-D_2(x_n^2+y_m^2)t}\int_0^t\left[D_2 a_m c_0^{(2)}x_n - \frac{(-1)^m}{\rho_2}g(t')\right]\mathrm{e}^{D_2(x_n^2+y_m^2)t'}\,\mathrm{d}t'. \qquad (24)$$

Function $g(t)$ is unknown in the expressions (18) and (24). Find it from the first contact condition of concentration equality on interface (11). In order to do it we perform inverse integral cosine transformation of concentration in both area $\overline{\Omega}_1$ by the formula (15) and area $\overline{\Omega}_2$ by (20). Then we obtain

$$\bar{c}_1(n,y,t) = \int_0^t\left(\left[D_1c_0^{(1)}x_n + \frac{g(t')}{\rho_1 L}\right].\mathrm{e}^{-D_1x_n^2(t-t')} + \frac{2g(t')}{\rho_1 L}\sum_{k=1}^{\infty}(-1)^k\cos(y_k y)\mathrm{e}^{-D_1(x_n^2+y_k^2)(t-t')}\right)\mathrm{d}t'; \qquad (25)$$

$$\bar{c}_2(n,y,t) = \int_0^t\left(\left[D_2c_0^{(2)}x_n - \frac{g(t')}{\rho_2 l}\right]\mathrm{e}^{-D_2x_n^2(t-t')} - \frac{2g(t')}{\rho_2 l}\sum_{m=1}^{\infty}(-1)^m\cos(y_m(y-L)) \times \mathrm{e}^{-D_2(x_n^2+y_m^2)(t-t')}\right)\mathrm{d}t'. \qquad (26)$$

Substitute the value $y = L$ in the expressions (25) and (26) and equate them multiplying functions $\bar{c}_i$ by corresponding coefficients of concentrating dependence of chemical potential k_i. As a result we obtain the following equation:

$$\begin{aligned}\int_0^t&\left[k_1c_0^{(1)}x_nD_1\mathrm{e}^{-D_1x_n^2(t-t')} + k_1\frac{g(t')}{\rho_1 L}\left\{\mathrm{e}^{-D_1x_n^2(t-t')} + 2\sum_{k=1}^{\infty}\mathrm{e}^{-D_1(x_n^2+y_k^2)(t-t')}\right\}\right]\mathrm{d}t'\\ &= \int_0^t\left[k_2c_0^{(2)}x_nD_2\mathrm{e}^{-D_2x_n^2(t-t')} - k_2\frac{g(t')}{\rho_2 l}\left\{\mathrm{e}^{-D_2x_n^2(t-t')} - 2\sum_{m=1}^{\infty}\mathrm{e}^{-D_2(x_n^2+y_m^2)(t-t')}\right\}\right]\mathrm{d}t'. \qquad (27)\end{aligned}$$

In order that a define integral of a nonperiodical function equals zero, it is enough that integral function equals zero. Then we obtain the equation for determination of unknown function $g(t')$

$$k_1\frac{g(t')}{L\rho_1}\left\{e^{-D_1x_n^2(t-t\prime)}+2\sum_{k=1}^{\infty}e^{-D_1(x_n^2+y_k^2)(t-t')}\right\}$$
$$+k_2\frac{g(t')}{l\rho_2}\left\{e^{-D_2x_n^2(t-t')}-2\sum_{m=1}^{\infty}e^{-D_2(x_n^2+y_m^2)(t-t')}\right\}$$
$$=k_2c_0^{(2)}x_nD_2e^{-D_2x_n^2(t-t')}-k_1c_0^{(1)}x_nD_1e^{-D_1x_n^2(t-t')}.$$

Whence we find

$$g(t')=\frac{x_n\left\{k_2c_0^{(2)}D_2e^{-D_2x_n^2(t-t')}-k_1c_0^{(1)}D_1e^{-D_1x_n^2(t-t')}\right\}}{\frac{k_1}{L\rho_1}e^{-D_1x_n^2(t-t')}+\frac{k_2}{l\rho_2}e^{-D_2x_n^2(t-t')}+2S_n(t-t')},\tag{28}$$

where

$$S_n(t-t')=\sum_{j=1}^{\infty}\left[\frac{k_1}{L\rho_1}e^{-D_1(x_n^2+(j\pi/L)^2)(t-t')}+\frac{(-1)^jk_2}{l\rho_2}e^{-D_2(x_n^2+(j\pi/l)^2)(t-t')}\right].$$

Remark the integral equation (27) has nonunique solution so far as it exists such functions $F(t')\neq 0$ that $\int_0^t F(t')\,dt'=0$. At the same time the original problem solution is unique independently of choice of solving integral equation manner since function $g(t')$ in the solutions c_1 and c_2 appears only under the integral of variable t'.

For obtaining the final solution of contact initial-boundary value problem (1)–(5) and (7) it remains to make inverse Fourier sine transformation of the expressions (25) and (26). Then we find

$$c_1(x,y,t)=c_0^{(1)}\left(1-\frac{x}{x_0}\right)-\frac{2}{x_0}\sum_{n=1}^{\infty}e^{-D_1x_n^2t}\sin(x_nx)\times\left\{\frac{c_0^{(1)}}{x_n}D_1-\frac{1}{\rho_1L}\int_0^t g(t')e^{D_1x_n^2t'}\,dt'+\frac{2}{\rho_1L}\sum_{k=1}^{\infty}(-1)^ke^{-D_1y_k^2t}\times\cos(y_ky)\int_0^t g(t')e^{D_1(x_n^2+y_k^2)t'}\,dt'\right\},\tag{29}$$

$$c_2(x,y,t)=c_0^{(2)}\left(1-\frac{x}{x_0}\right)-\frac{2}{x_0}\sum_{n=1}^{\infty}e^{-D_2x_n^2t}\sin(x_nx)\times\left\{\frac{c_0^{(2)}}{x_n}D_2-\frac{1}{\rho_2l}\int_0^t g(t')e^{D_2x_n^2t'}\,dt'+\frac{2}{\rho_2l}\sum_{m=1}^{\infty}(-1)^me^{-D_2y_m^2t}\times\cos(y_my)\int_0^t g(t')e^{D_2(x_n^2+y_m^2)t'}\,dt'\right\},\tag{30}$$

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

4. Relation between problems of diffusion in horizontally regular structure and heterodiffusion by two ways. Dimensionless form

Average the functions of admixture concentration $c_1(x,y,t)$ and $c_2(x,y,t)$ over all width of the separated body element $[0;L+l]$:

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

Then such averaged functions have to satisfy the following equations:

$$\frac{\partial\hat{c}_1}{\partial t}=D_1\frac{\partial^2\hat{c}_1}{\partial x^2}+\frac{D_1}{L+l}\frac{\partial c_1}{\partial y}\Big|_{y=L},$$
$$\frac{\partial\hat{c}_2}{\partial t}=D_2\frac{\partial^2\hat{c}_2}{\partial x^2}+\frac{D_2}{L+l}\frac{\partial c_2}{\partial y}\Big|_{y=L}.$$

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

$$\rho_1D_1\frac{\partial c_1}{\partial y}\Big|_{y=L}=\theta_2\Delta\mu_2-\theta_1\Delta\mu_1|_{y=L},$$
$$\rho_2D_2\frac{\partial c_2}{\partial y}\Big|_{y=L}=\theta_1\Delta\mu_1-\theta_2\Delta\mu_2|_{y=L},$$

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

$$\frac{\partial\hat{c}_1}{\partial t}=D_1\frac{\partial^2\hat{c}_1}{\partial x^2}+\frac{1}{\rho_1(L+l)}(\theta_2\Delta\mu_2-\theta_1\Delta\mu_1)|_{y=L},$$
$$\frac{\partial\hat{c}_2}{\partial t}=D_2\frac{\partial^2\hat{c}_2}{\partial x^2}-\frac{1}{\rho_2(L+l)}(\theta_2\Delta\mu_2-\theta_1\Delta\mu_1)|_{y=L}.\tag{32}$$

So long as $\Delta\mu_i|_{y=L}=k_ic_i|_{y=L}$, the set of Eqs. (32) can be written in the form

$$\frac{\partial\hat{c}_1}{\partial t}=D_1\frac{\partial^2\hat{c}_1}{\partial x^2}+\frac{1}{\rho_1(L+l)}(k_2\theta_2c_2-k_1\theta_1c_1)|_{y=L},$$
$$\frac{\partial\hat{c}_2}{\partial t}=D_2\frac{\partial^2\hat{c}_2}{\partial x^2}-\frac{1}{\rho_2(L+l)}(k_2\theta_2c_2-k_1\theta_1c_1)|_{y=L}.$$

If the condition $\frac{1}{L+l}c_i(x,L,t)\approx\hat{c}_i(x,t)$ takes place then we obtain a coupled set of differential equations of admixture heterodiffusion by two ways [1,2,12]

$$\rho_1\frac{\partial\hat{c}_1}{\partial t}=\rho_1D_1\frac{\partial^2\hat{c}_1}{\partial x^2}-\bar{k}_1\hat{c}_1+\bar{k}_2\hat{c}_2,$$
$$\rho_2\frac{\partial\hat{c}_2}{\partial t}=\rho_2D_2\frac{\partial^2\hat{c}_2}{\partial x^2}-\bar{k}_1\hat{c}_1+\bar{k}_2\hat{c}_2,\tag{33}$$

where $\bar{k}_i=\theta_ik_i$ ($i=1,2$) are coefficients of intensity of particle transition between different diffusion ways.

Thus, subject to the equality of admixture fluxes and linear combinations of chemical potentials on a contact boundary by means of averaging concentrations over

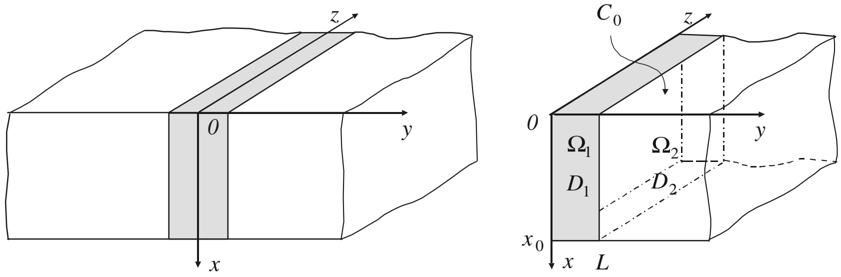

Fig. 2. Diffusion in a polycrystal along grain boundary.

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 we can introduce a natural dimensionless form for such a problem [12]:

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

Take into consideration the dimensionless space variable $\eta = (k_2/D_1)^{1/2}y$. Then the contact initial boundary value problem (1)–(5) and (7) can be presented in a dimensionless form:

$$\frac{\partial c_1}{\partial \tau} = \frac{\partial^2 c_1}{\partial \xi^2} + \frac{\partial^2 c_1}{\partial \eta^2}, \quad \xi, \eta \in \omega_1 =]0; \xi_0[\times]0; \Lambda[, \tag{35}$$

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

$$\begin{aligned} &c_1(\xi,\eta,\tau)|_{\tau=0} = c_2(\xi,\eta,\tau)|_{\tau=0} = 0,\\ &c_1(\xi,\eta,\tau)|_{\xi=0} = c_0^{(1)}, \quad c_2(\xi,\eta,\tau)|_{\xi=0} = c_0^{(2)},\\ &c_1(\xi,\eta,\tau)|_{\xi=\xi_0} = c_2(\xi,\eta,\tau)|_{\xi=\xi_0} = 0;\\ &\left.\frac{\partial c_1(\xi,\eta,\tau)}{\partial \eta}\right|_{\eta=0} = \left.\frac{\partial c_2(\xi,\eta,\tau)}{\partial \eta}\right|_{\eta=\Lambda+\lambda} = 0; \end{aligned} \tag{37}$$

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

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

5. Fisher problem as a particular case of diffusion problem in horizontally periodical structure

If in the relationships (1)–(5) and (7) we tend the width of area Ω_2 to infinity $l \to \infty$ ($L \neq 0$) then we obtain Fisher problem [4,5] for a layer modelling diffusion in a polycrystal along grain boundary. That is admixture diffusion in a semi-infinite solid in which a thin plate was put into so as its plane is perpendicular to the body surface (see Fig. 2). Assume that concentration of diffuser conserves its constant values on a free sample surface and diffusion coefficient D_1 in a plate (that conforms to a grain boundary) is much greater then D_2 characterizing mass transfer in the remaining body [4].

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

$$\begin{aligned} &\lim_{l\to\infty} c_1(x,y,t)\\ &\quad = c_0^{(1)}\left(1 - \frac{x}{x_0}\right) - \frac{2}{x_0}\sum_{n=1}^{\infty}\sin(x_n x)e^{-D_1 x_n^2 t}\\ &\quad\times\left(\frac{c_0^{(1)}}{x_n}D_1 - \frac{1}{L\rho_1}\int_0^t \hat{g}(t')e^{D_1 x_n^2 t'}\,dt'\right.\\ &\quad\left.+\frac{2}{\rho_1 L}\sum_{k=1}^{\infty}(-1)^k e^{-D_1 y_k^2 t}\cos(y_k y)\int_0^t \hat{g}(t')e^{D_1(x_n^2+y_k^2)t'}\,dt'\right), \end{aligned} \tag{39}$$

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

where

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

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

Note that the expression (40) for admixture concentration in area Ω_2 is identical to solution of one-dimensional diffusion problem for a layer with diffusion coefficient D_2 and initial and boundary conditions (3) and (4) that corresponds the results mentioned in [4].

6. Numerical analysis of admixture concentration behaviour in a body with horizontally regular structure

Illustration of admixture concentration distributions in a layer with horizontally periodical structure computed by formulae (29), (30) is presented in Figs. 3–10. Numerical calculations have been done in the dimensionless variables τ, ξ, η introduced by (34). The problem coefficients have been taken $\xi_0 = 10$; $\Lambda = 1$, $\lambda = 0.1$, $d = D_2/D_1 = 0.01$, $\rho_2/\rho_1 = 1.5$, $c_0^{(1)}/c_0^{(2)} = 0.1$. Distributions of admixture concentration along $O\xi$-axis in different time moments τ=1; 5; 10; 20; 100 (curves 1–5 correspondingly) are shown in Fig. 3 in the middle of area Ω_1, i.e. at $\eta = 0.5$, and Fig. 4 at $\eta = 1.05$ (middle of area Ω_2) for $\bar{k}_1/\bar{k}_2 = 10$. Fig. 5 ($\eta = 0.5$) and Fig. 6 ($\eta = 1.05$) illustrate behaviour of concentration function for different values of ratio $\bar{k}_1/\bar{k}_2 = 100$; 10; 2; 0.5; 0.1 (curves 1–5) in dimensionless moment $\tau = 10$. Fig. 7 ($\eta = 0.5$) and Fig. 8 ($\eta = 1.05$) show $c(\xi, \eta, \tau)/c_0^{(2)}$ in dependence on ratio of diffusion coefficients $d = 0.01$; 0.1; 0.5 (curves 1–3) at $\bar{k}_1/\bar{k}_2 = 10$, $\tau = 10$.

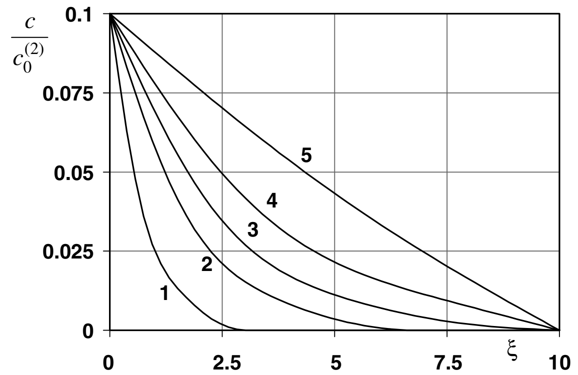

Fig. 3. Distributions of admixture concentration along depth in the middle of area Ω_1.

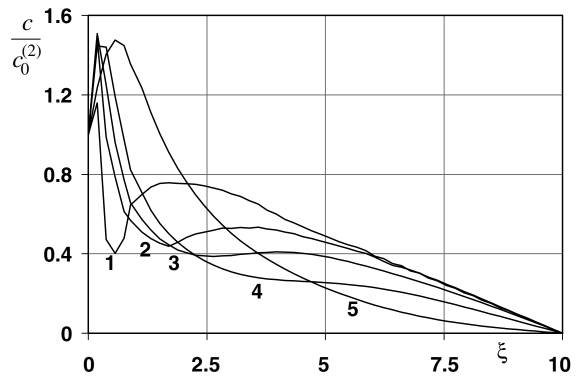

Fig. 4. Distributions of admixture concentration along depth in the middle of area Ω_2.

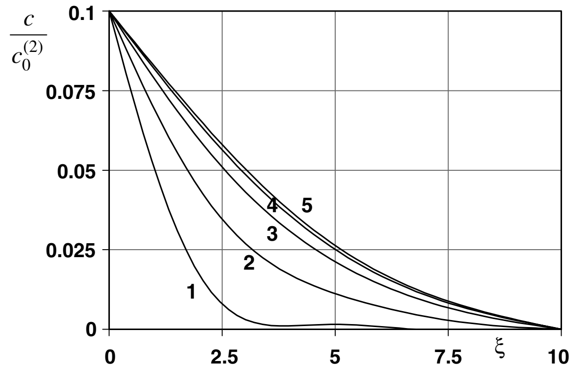

Fig. 5. Admixture concentration for different values of ratio of particle intertransitions intensity coefficients k_1/k_2 in the middle of area Ω_1.

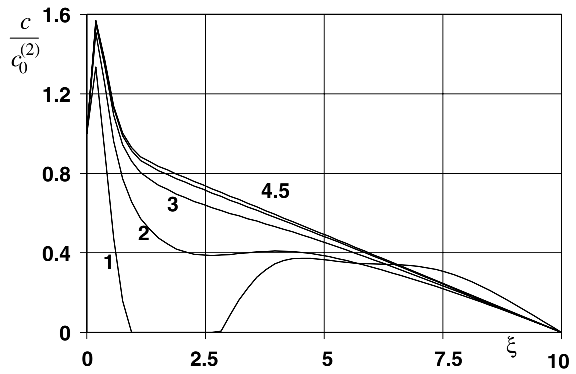

Fig. 6. Admixture concentration for different values of ratio of particle intertransitions intensity coefficients k_1/k_2 in the middle of area Ω_2.

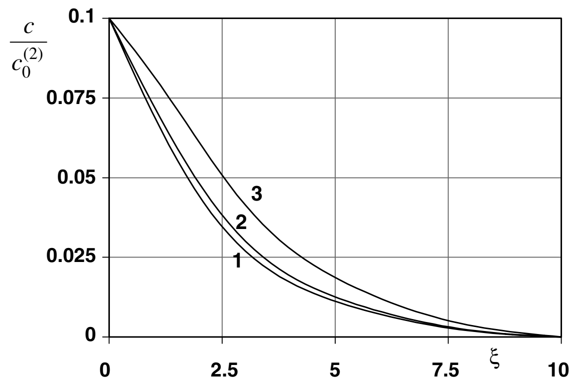

Fig. 7. Dependence of admixture concentration on ratio of diffusion coefficients $d = D_2/D_1$ in the middle of area Ω_1.

Graphs of admixture concentration along $O\eta$-axis, i.e. on width of the separated body element, are demonstrated in Figs. 9 and 10. Fig. 9 illustrates concentration

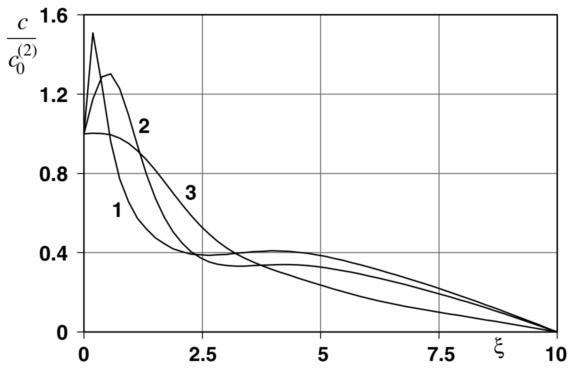

Fig. 8. Dependence of admixture concentration on ratio of diffusion coefficients d in the middle of area Ω_2.

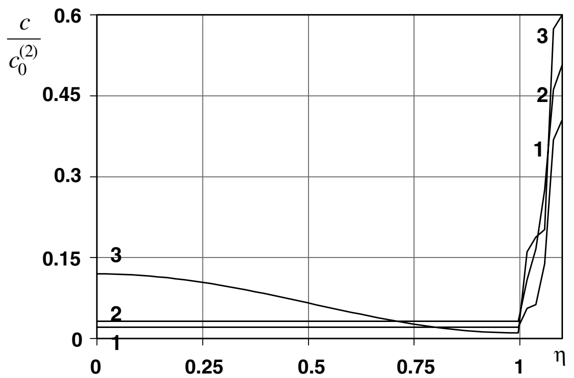

Fig. 9. Distributions of admixture concentration along body element width for different times.

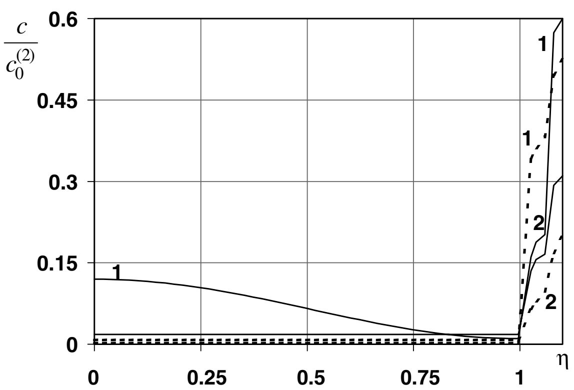

Fig. 10. Concentration distributions along body element width for different values of ratio of diffusion coefficients d.

in different times $\tau = 1; 5; 10$ (curves 1–3) at depth $\xi = 1$ for $d = 0.01$, $\bar{k}_1/\bar{k}_2 = 10$. Concentration is shown in Fig. 10 for different values of ratio of diffusion coefficients $d = 0.1; 0.01$ (curves 1 and 2). Here full lines mark the function $c(\xi, \eta, \tau)/c_0^{(1)}$ under $\bar{k}_1/\bar{k}_2 = 10$ and dashed lines identify them under $\bar{k}_1/\bar{k}_2 = 0.1$ at $\tau = 1$.

Let us note that behaviour of admixture concentration function along layer depth is substantially different in areas Ω_1 and Ω_2. So concentration distributions in region Ω_1 with quick diffusion coefficient are similar to ones in a homogeneous layer (see Figs. 3, 5 and 7). At the same time in area Ω_2 with slow diffusion coefficient there is subsurface increase of concentration. Such situation is characteristic of heterodiffusion by two ways (see Figs. 4, 6, and 8). But in this case it is possible to occur the second local maximum at the body depth for both small times and much more severe transition admixture particles from region with quick diffusion coefficient into area with slow one (see Fig. 6, curves 1 and 2).

7. Mass fluxes in a layer with horizontally periodical structure

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

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

Substituting the corresponding expressions for admixture concentrations (29), (30) into (41) we obtain the following formulae for mass fluxes through per unit of surface area $x = x^*$ in area Ω_1

$$J_*^{(1)}(t) = \frac{D_1}{x_0}\Bigg[C_0^{(1)} + 2\sum_{n=1}^{\infty} e^{-D_1 x_n^2 t} \cos(x_n x^*) \Bigg\{ c_0^{(1)} D_1 - \frac{x_n}{\rho_1 L} \times \int_0^t g(t') e^{D_1 x_n^2 t'} dt' + \frac{2x_n}{\rho_1 L} \sum_{k=1}^{\infty} (-1)^k e^{-D_1 y_k^2 t} \cos(y_k y) \times \int_0^t g(t') e^{D_1 (x_n^2 + y_k^2) t'} dt' \Bigg\}\Bigg], \tag{42}$$

in area Ω_2

$$J_*^{(2)}(t) = \frac{D_2}{x_0}\Bigg[c_0^{(2)} + 2\sum_{n=1}^{\infty} e^{-D_2 x_n^2 t} \cos(x_n x^*) \Bigg\{ c_0^{(2)} D_2 - \frac{x_n}{\rho_2 l} \times \int_0^t g(t') e^{D_2 x_n^2 t'} dt' + \frac{2x_n}{\rho_2 l} \sum_{m=1}^{\infty} (-1)^m e^{-D_2 y_m^2 t} \cos(y_m y) \times \int_0^t g(t') e^{D_2 (x_n^2 + y_m^2) t'} dt' \Bigg\}\Bigg]. \tag{43}$$

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

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

in area Ω_2

$$J_0^{(2)}(t) = \frac{D_2}{x_0}\left[c_0^{(2)} + 2\sum_{n=1}^{\infty}(-1)^n \mathrm{e}^{-D_2 x_n^2 t}\left\{c_0^{(2)} D_2 - \frac{x_n}{\rho_2 l} \times \int_0^t g(t')\mathrm{e}^{D_2 x_n^2 t'}\,\mathrm{d}t' + \frac{2x_n}{\rho_2 l}\sum_{m=1}^{\infty}(-1)^m \mathrm{e}^{-D_2 y_m^2 t}\cos(y_m y) \times \int_0^t g(t')\mathrm{e}^{D_2(x_n^2+y_m^2)t'}\,\mathrm{d}t'\right\}\right].$$

In the same way we can find mass fluxes through any vertical surface $y = y^*$.

8. Conclusion

In this work for obtaining exact analytical solutions of contact initial-boundary value problems of mass transfer it was proposed new method based on application of integral transformations apart in contacting areas. Determination of analytical expressions for admixture concentration allows to find mass fluxes through per unit of the given surface area. Obtaining the exact solution of such problem gives also an opportunity to find exact solutions for particular practically important Fisher problem.

The conditions have been determined when relation between diffusion problem in a body with horizontally periodical structure and problem of one-dimensional heterodiffusion by two ways exists. It gives a possibility to introduce natural dimensionless form for a problem of mass transfer in horizontally regular structures too. Remark that change to a heterodiffusion problem exists only under conditions of nonideal mass contact. If ideal contact conditions realize then we obtain change to the model of "noninteracting fluxes", i.e. mass transfer by two ways not accompanied by particle intertransitions from one migration way into another.

Finally, note that the proposed method for constructing exact solution of contact initial-boundary value problems does not use condition on sizes of contacting areas. So it can be suitable both for bodies with comparable sizes of contacting regions and in the cases when one area width is much greater (or smaller) then another.

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