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On Solving the Problems of Nonstationary Diffusion in Layered Environments

Sergey Vladimirovich Vendin[1*]

[1]Department of Electrical and Electrotechnology in AIC, Faculty of Engineering, Federal State Budgetary Educational Institution of Higher Education "Belgorod State Agricultural University named after V. Gorin", 1 Vavilova Street, Majskij village, Belgorod Region, 308503, Russian Federation.
(Corresponding Author)[*]

Abstract

The issues of nonstationary diffusion in multilayer objects are considered. A solution of the homogeneous boundary problem with third-type nonstationary boundary conditions on the object surface and fourth-type conjugation boundary conditions on mating surfaces is proposed. The following is at the base of the solution: Fourier method of variables partition into proper functions of the problem and Duhamel integral. The proposed form of solution has an explicit form, and due to the recurrent form of the basic relations recording it can be useful at numerical calculations.

Keywords: boundary problem, nonstationary diffusion equations, multilayer object, nonstationary third-type boundary conditions, nonstationary fourth-type boundary conditions.

Many important practical problems of the nonstationary diffusion calculation (the second Fick law) [1, p. 478; 2, p. 752] in multilayer objects can be considered as one-dimensional. Previously the author proposed an analytical solution for the homogeneous nonstationary problem of heat conductivity in multilayer objects at third-type stationary boundary conditions [3-5], and third-type nonstationary boundary conditions [6]. The nonstationary diffusion equation solution can be obtained in the same way with account for boundary conditions and observation of the orthogonality conditions of the proper functions of the problem.

The solution of homogeneous boundary problem with third-type nonstationary boundary conditions on the object surface and fourth-type conjugation boundary conditions on mating surfaces is given below.

In the general case, the mathematical setting of the one-dimensional nonstationary diffusion for multilayer objects can be determined by the following system of differential equations:

$$\frac{\partial C_i(r,t)}{\partial t} = D_i \nabla^2 C_i(r,t), \quad x_{i-1} \le r \le x_i,\ i = 1, 2, \ldots n, \qquad (1)$$

where $C_i(r,t)$, D_i, – material concentration and diffusion coefficients in the i-th layer, respectively; x_0, x_n – coordinates of the upper and lower geometrical (free) surfaces of the object, respectively.

Let us determine the boundary conditions on the free surfaces $r = x_o$, $r = x_n$ as third-type nonstationary boundary conditions. In this case, we record the following:

$$\left[C_1(r,t) + h_1 \frac{\partial C_1(r,t)}{\partial r}\right]_{r=x_0} = \varphi_1(t),$$

$$\left[C_n(r,t) + h_2 \frac{\partial C_n(r,t)}{\partial r}\right]_{r=x_n} = \varphi_2(t). \qquad (2)$$

The boundary conditions of concentration fields and concentration flows conjugation on the layers interfaces in the general case are determined by the following expressions:

$$\left| K_i C_i(r,t) = K_{i+1} C_{i+1}(r,t) \right|_{r=x_i},$$

$$\left| D_i \frac{\partial C_i(r,t)}{\partial r} = D_{i+1} \frac{\partial C_{i+1}(r,t)}{\partial r} \right|_{r=x_i} \quad i = 1, 2, \ldots n-1, \qquad (3)$$

where K_i is the i-th layer solubility constant.

The initial distribution of concentrated fields on each layer has the form:

$$C_i(r,0) = f_i(r), \quad i = 1, 2, \ldots n. \qquad (4)$$

If we represent the searched solution of the problem as the sum of

$$C_i(r,t) = f_i(r) + v_i(r,t), \qquad (5)$$

then the problem is converged to the determination of the functions $v_i(r,t)$, which are the solution of the problem with zero initial conditions $v_i(r,0) = 0$ and satisfy the equations (1)-(3).

The solution of the problem of time-dependent nonhomogeneous boundary conditions can be determined by the Duhamel integral [7, p. 550; 8, p. 835]:

$$v_i(r,t) = \int_0^t \frac{\partial}{\partial t} \dot{v}_i(r,\tau,t-\tau)\, d\tau, \text{ at } t > 0, \qquad (6)$$

where $\dot{v}_i(r,\tau,t)$ is the problem solution at the condition that τ is a parameter.

In accordance with the found solution, the functions $v_i(r,t)$ have the form:

$$v_i(r,t) = \sum_{m=0}^{\infty}\left[-\mu_{i,m}^2 D_i \int_0^t A_m(\tau)\exp(\mu_{i,m}^2 D_i \tau)d\tau\right]\dot{F}_{i,m}(\mu_{i,m} r)\exp(-\mu_{i,m}^2 D_i t), \quad (7)$$

where $\dot{F}_{i,m}(\mu_{i,m} r)$ are proper functions of the problem

$$\dot{F}_{i,m}(\mu_{i,m} r) = \left[\prod_{k=1}^{i} Z_k\right]\times\left[Y_1(\mu_{i,m} r) + B_{i,m} Y_2(\mu_{i,m} r)\right], \ \text{i = 1,2,…n} \quad (8)$$

$$B_{1,m} = -\frac{Y_1(\mu_{1,m} x_0) + h_1 Y_1'(\mu_{1,m} x_0)}{Y_2(\mu_{1,m} x_0) + h_1 Y_2'(\mu_{1,m} x_0)} \quad (9)$$

$$B_{i,m} = -\frac{\frac{D_i}{K_i}\times\frac{Y_1'(\mu_{i,m} x_{i-1})}{Y_1(\mu_{i,m} x_{i-1})} - \frac{D_{i-1}}{K_{i-1}}\times\frac{Y_1'(\mu_{i-1,m} x_{i-1}) + B_{i-1} Y_2'(\mu_{i-1,m} x_{i-1})}{Y_1(\mu_{i-1,m} x_{i-1}) + B_{i-1} Y_2(\mu_{i-1,m} x_{i-1})}}{\frac{D_i}{K_i}\times\frac{Y_2'(\mu_{i,m} x_{i-1})}{Y_2(\mu_{i,m} x_{i-1})} - \frac{D_{i-1}}{K_{i-1}}\times\frac{Y_1'(\mu_{i-1}, m x_{i-1}) + B_{i-1} Y_2'(\mu_{i-1,m} x_{i-1})}{Y_1(\mu_{i-1,m} x_{i-1}) + B_{i-1} Y_2(\mu_{i-1,m} x_{i-1})}}\times\frac{Y_1(\mu_{i,m} x_{i-1})}{Y_2(\mu_{i,m} x_{i-1})} \quad (10)$$

i = 2,3,…n.

$$Z_1 = 1; \ Z_i = \frac{K_{i-1}}{K_i}\times\frac{Y_1(\mu_{i-1,m} x_{i-1}) + B_{i-1} Y_2(\mu_{i-1,m} x_{i-1})}{Y_1(\mu_{i,m} x_{i-1}) + B_i Y_2(\mu_{i,m} x_{i-1})}, \ \text{i = 2,3,…n}, \quad (11)$$

$\mu_{i,m} = \mu_{n,m}\sqrt{D_n / D_i}$, $\mu_{n,m}$ – proper numbers of the problem determined according to the equation:

$$Y_1(\mu_{n,m} x_n) + h_2 Y_1'(\mu_{n,m} x_n) + B_{n,m}[Y_2(\mu_{n,m} x_n) + h_2 Y_2'(\mu_{n,m} x_n)] = 0, \ \text{m = 0,1,2,…} \quad (12)$$

$$A_m(\tau) = -\left[\sum_{i=1}^{n} K_i \int_{x_{i-1}}^{x_i} \psi_i(r,\tau) G(r) \dot{F}_{i,m}(\mu_{i,m} r) dr\right] / \sum_{i=1}^{n} \dot{J}_i^2, \quad (13)$$

$$\psi_i(r,\tau) = \varphi_1(\tau) + \dot{\alpha}_i(\tau)[\varphi_2(\tau) - \varphi_1(\tau)]\times[\xi(r) + \dot{\beta}_i(\tau)], \quad (14)$$

$$\dot{\beta}_1(\tau) = -[\xi(x_0) + h_1 \xi'(x_0)], \ \dot{\beta}_i(\tau) = \frac{D_i K_{i-1}}{D_{i-1} K_i}\times\left[\xi(x_{i-1}) + \dot{\beta}_{i-1}\right] - \xi(x_{i-1}), \ \text{i = 2,3,…n} \quad (15)$$

$$\dot{\alpha}_i = \frac{D_n}{D_i}\times\frac{1}{\xi(x_n) + \dot{\beta}_n(\tau) + h_2 \xi'(x_n)}, \ \text{i = 1, 2,…n.} \quad (16)$$

$$\dot{J}_i^2 = K_i \int_{x_{i-1}}^{x_i} G(r) \dot{F}_{i,m}^2(\mu_{i,m} r) dr. \quad (17)$$

The weight function $G(r)$, as well as the certain form of the functions $\xi(r)$ and $\dot{F}_i(\mu_i r)$, is determined by the expressions:

a) The Cartesian (rectangular) coordinate system:

$$G(r) = 1, \xi(r) = r, Y_1(\mu_i r) = \sin(\mu_i r), Y_2(\mu_i r) = \cos(\mu_i r). \quad (18)$$

b) Spherical coordinate system:

$$G(r)=r^2, \xi(r)=\frac{1}{r}, Y_1(\mu_i r)=\frac{1}{r}\sin(\mu_i r), Y_2(\mu_i r)=\frac{1}{r}\cos(\mu_i r). \quad (19)$$

c) Cylindrical coordinate system:

$$G(r)=r, \xi(r)=\ln r, Y_1(\mu_i r)=J_0(\mu_i r), Y_2(\mu_i r)=N_0(\mu_i r). \quad (20)$$

Important comment:

Sometimes, when solving the problems for a solid ball or cylinder, the obtained solution requires boundaries in the center of the ball or on the cylinder axis. Then, the lower and the upper boundary conditions are written in the following form:

$$\left[\frac{\partial C_1(r,t)}{\partial r}\right]_{r=x_0}=0,$$

$$\left[C_n(r,t)+h_2\frac{\partial C_n(r,t)}{\partial r}\right]_{r=x_n}=\varphi_2(t) \quad (21)$$

In such case, in the obtained solutions for multilayer objects we should assume that

$$B_{1,m}=0,\ \psi_i(r,\tau)=\varphi_2(\tau)\text{ , i=1,2...n} \quad (22)$$

and then, all the calculations are made in accordance with the main solution.

Thus, we have obtained the general solution for the boundary homogeneous problem with third-type boundary conditions. The proposed form of solution has an explicit form, and due to the recurrent form of the basic relations recording it can be useful at numerical calculations and analysis of the nonstationary diffusion kinetics in multilayer environments.

Various particular solutions of such problems can be immediately recorded with account for the boundary conditions (2), as well as the expressions (4), (5), (7) and (21)-(22).

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