# ON THE SOLUTION OF EQUATIONS OF NONSTATIONARY DIFFUSION IN MULTILAYER ACTIVE MEDIA WITH LINEAR INTERACTIONS

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## Abstract

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# ON THE SOLUTION OF EQUATIONS OF NONSTATIONARY DIFFUSION IN MULTILAYER ACTIVE MEDIA WITH LINEAR INTERACTIONS

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Problems in the theory of diffusion in media interacting with diffusing substances have, over the past two decades, found wide application in scientific and engineering practice. The importance of such problems in the study of chain processes is well known. Most such problems have been solved as applied to simple classical domains—a plate, cylinder, sphere, and parallelepiped—under the assumption that the interaction is described by a linear term, i.e., solutions were sought for equations of the form

$$u'_t = D\Delta u + ku \tag{1}$$

under various boundary and initial conditions. Equation (1) describes diffusion (or heat conduction) in media containing sources ($k > 0$) or sinks ($k < 0$), whose productivity is proportional to the concentration (respectively, temperature).

Of special interest for practical applications are such problems considered for multilayer media, i.e., for domains with a discontinuous diffusion coefficient $D$ and a discontinuous coefficient $k$. In general form, solutions of such problems can be obtained by the operational method using Green' s functions ([1]), or by means of finite integral transformations of Grinberg ([2]), which make it possible to obtain solutions for anisotropic (with respect to $D$) domains in the most general form; however, solutions presented in this form are extremely cumbersome, and obtaining final numerical results is very laborious and difficult.

Diffusion fluxes in active media in the linear approximation and for simple domains were also considered in works ([3–5]), in which, however, the question of multilayer domains was not touched upon. In works ([6–8]) a simple method was given for the operational solution of heat-conduction equations without sources in multilayer media, making it possible to obtain final numerical results quite rapidly for the most widely applicable class of problems with initial conditions

Fig. 1

Figure 1: Fig. 1

of the type $u_j|_{t=0} = \text{const}$ ($j$ is the layer number). This method admits a natural generalization to the case of linear equations of the form (1).

Applying substitutions of the form $u_j = U_j e^{k_j t}$ for each of the media, or passing directly to the Laplace transforms of systems of the form (1), we obtain systems of equations for determining the unknown coefficients—functions of the operational variable $s$—which are structurally analogous to the equations for systems without sources. In this case the general structure of the principal determinant is preserved, and therefore all conclusions concerning the characteristic roots—the roots of the denominators of the transforms of the solutions—remain valid.

At the same time, we obtain a simple and convenient approach to the solution of numerous problems of diffusion kinetics in multilayer active media, especially interesting for the analysis of transfer processes in complex

biological objects. Examples that may be mentioned include: the establishment of membrane equilibria, the dynamics of the establishment of the action potential of nerve fibers, the mechanism of propagation of synaptic mediators, etc.

Taking into account the range of applications of this method, we shall present its essence as applied to systems of type (I) for plane multilayer media, for which the principal stages of the solution are most transparent, and the number of possible applications is sufficiently large.

A schematic representation of the medium under consideration is given in Fig. 1. The medium consists of $n$ layers of different thicknesses $\delta_j$ and is bounded either by "impermeable" walls, corresponding in real problems to the external boundaries of the closed systems under consideration, or the external left boundary is identified with the right one, if a process is considered in a medium consisting of repeated cyclic groupings of layers of identical structure. If the medium is considered as an "open" system (in the thermodynamic sense), then such problems can also be reduced to problems with impermeable walls, if the outer layers are identified with the medium external to the system.

**Fig. 1**

The concentrations of the diffusing substance in the $j$-th layer ($u_j$) are assumed to satisfy the equations

$$\partial u_j/\partial t = D_j \partial^2 u_j/\partial x^2 - k_j u_j \qquad (j = 1, \dots, n), \tag{1}$$

where $u_j = u_j(x, t; D_j k_j)$, with boundary conditions on the "internal" boundaries of the layers

$$u_j\big|_{x=l_j} = u_{j+1}\big|_{x=l_j}, \qquad D_j(u_j)'_x\big|_{x=l_j} = D_{j+1}(u_{j+1})'_x\big|_{x=l_j}, \tag{2}$$

where $l_j$ is the right boundary of the $j$-th layer. On the external boundaries we impose the conditions of "impermeability"

$$(u_1)'_x\big|_{x=0} = 0; \qquad (u_n)'_x\big|_{x=l_n} = 0, \tag{3}$$

i.e., we restrict ourselves to consideration of "internal" problems.

The initial conditions for the most part have the form

$$u_j\big|_{t=0} = c_j = \text{const} \qquad (l_{j-1} < x < l_j), \tag{4}$$

i.e., the initial concentrations in each of the layers are constant.

As indicated above, one may either pass directly to the Laplace transforms of system (1)–(4), or first carry out a substitution. We shall use the second path. Put

$$u_j = U_j e^{-k_j t}. \tag{5}$$

As a result of the substitution, system (1) is transformed into the system:

$$(U_j)'_t = D_j(U_j)''_{xx} \qquad (j = 1, \dots, n) \tag{1'}$$

with boundary conditions

$$U_j e^{-k_j t}\big|_{l_j} = U_{j+1} e^{-k_{j+1} t}\big|_{l_j};$$

$$D_j(U_j)'_x e^{-k_j t}\big|_{l_j} = D_{j+1}(U_{j+1})'_x e^{-k_{j+1} t}\big|_{l_j}, \tag{2'}$$

$$(U_1)'_x\big|_{x=0} = (U_n)'_x\big|_{x=l_n} = 0 \tag{3'}$$

and the former initial conditions

$$U_j\big|_{t=0} = c_j \qquad (j = 1, \dots, n). \tag{4'}$$

The general solutions of equations (1′) in the domain of Laplace transforms, as is well known, may be written in the form

$$\overline{U}_j(x,s) = \frac{c_j}{s} + A_j \operatorname{ch}\left(\sqrt{\frac{s}{D_j}}\,x\right) + B_j \operatorname{sh}\left(\sqrt{\frac{s}{D_j}}\,x\right), \tag{6}$$

where $A_j = A_j(s)$, $B_j = B_j(s)$, whence, in particular,

$$(\overline{U})'_x = A_j\sqrt{\frac{s}{D_j}} \operatorname{sh}\left(\sqrt{\frac{s}{D_j}}\,x\right) + B_j\sqrt{\frac{s}{D_j}} \operatorname{ch}\left(\sqrt{\frac{s}{D_j}}\,x\right), \tag{7}$$

and the boundary conditions in the transform domain are transformed (by the damping theorem) into the conditions

$$\overline{U}_j(x; s+k_j)\big|_{l_j} = \overline{U}_{j+1}(x; s+k_{j+1})\big|_{l_j},$$

$$D_j\frac{\partial}{\partial x}\overline{U}_j(x; s+k_j)\big|_{l_j} = D_{j+1}\frac{\partial}{\partial x}\overline{U}_{j+1}(x; s+k_{j+1})\big|_{l_j}, \tag{8}$$

$$\left.\frac{\partial \overline{U}_1}{\partial x}\right|_{x=0} = \left.\frac{\partial \overline{U}_n}{\partial x}\right|_{x=l_n} = 0.$$

In what follows, to shorten the notation, we shall apply a method of abbreviated notation analogous to that proposed in ([6]). Namely, put

$$\left.\begin{matrix}\operatorname{sh}\\ \operatorname{ch}\end{matrix}\right\}\left(\sqrt{\frac{s+k_j}{D_j}}\,x\right)\Bigg|_{x=l_j} = \left.\begin{matrix}\operatorname{sh}\\ \operatorname{ch}\end{matrix}\right\}\left(\sqrt{\frac{s+k_j}{D_j}}\,l_j\right) = \left\{\begin{matrix}\operatorname{sh}_{jj},\\ \operatorname{ch}_{jj};\end{matrix}\right.$$

$$\left.\begin{matrix}\operatorname{sh}\\ \operatorname{ch}\end{matrix}\right\}\left(\sqrt{\frac{s+k_{j+1}}{D_{j+1}}}\,x\right)\Bigg|_{x=l_j} = \left.\begin{matrix}\operatorname{sh}\\ \operatorname{ch}\end{matrix}\right\}\left(\sqrt{\frac{s+k_{j+1}}{D_{j+1}}}\,l_j\right) = \left\{\begin{matrix}\operatorname{sh}_{j+1,j},\\ \operatorname{ch}_{j+1,j};\end{matrix}\right.$$

i.e., by the first index we shall denote the number of the layer, and by the second, the number of the layer boundary. Then, substituting (6) and (7) into (8), we obtain, for the $j$-th internal boundary, two equations:

$$A_j \operatorname{ch}_{jj} + B_j \operatorname{sh}_{jj} + \frac{c_j}{s+k_j} = A_{j+1}\operatorname{ch}_{j+1,j} + B_{j+1}\operatorname{sh}_{j+1,j} + \frac{c_{j+1}}{s+k_{j+1}}; \tag{9}$$

$$D_j\left(A_j\sqrt{\frac{s+k_j}{D_j}}\operatorname{sh}_{jj} + B_j\sqrt{\frac{s+k_j}{D_j}}\operatorname{ch}_{jj}\right) =$$

$$= D_{j+1} \left( A_{j+1} \sqrt{\frac{s + k_{j+1}}{D_{j+1}}} \operatorname{sh}_{j+1,j} + B_{j+1} \sqrt{\frac{s + k_{j+1}}{D_{j+1}}} \operatorname{ch}_{j+1,j} \right) \tag{10}$$

and for the external boundaries

$$B_1 = 0; \tag{11}$$

$$A_n \sqrt{\frac{s}{D_n}} \operatorname{sh}_{nn} + B_n \sqrt{\frac{s}{D_n}} \operatorname{ch}_{nn} = 0. \tag{12}$$

The system of equations (9)—(12) contains $2n$ equations for the unknown functions of the variable $s$—the coefficients $A_j$ and $B_j$ $(j = 1, 2, \dots, n)$. Its solutions, as is well known, can be written through the determinant of the system and the partial determinants corresponding to each of the unknowns. As a result, the transforms of the solutions of the equations—formulas (6)—take the form:

$$\overline{U}_j(x, s) = \frac{c_j}{s} + \frac{\Delta_{A_j}}{\Delta} \operatorname{ch} \left( x \sqrt{\frac{s}{D_j}} \right) + \frac{\Delta_{B_j}}{\Delta} \operatorname{sh} \left( x \sqrt{\frac{s}{D_j}} \right), \tag{13}$$

where $\Delta$ is the determinant of the system (9)—(12), and $\Delta_{A_j}$ and $\Delta_{B_j}$ are the determinants $\Delta$ in which the columns corresponding to $A_j$ and $B_j$ are replaced by the columns of the free terms.

It is easy to see that, despite a certain complication of the system (9)—(12) in comparison with the systems considered in ([6]), due to a partial replacement of the operational variable $s$ by $s + k_j$ (a complete replacement of $s$ by $s + k$ for $k = \text{const}$ would make it possible immediately to use the theorem

decay and immediately write the solution), the main conclusions on the representability of the solution of the expansion theorems remain valid. In addition, one can still use, for computing the determinant $\Delta$, formulas for the sh and ch of differences of arguments, which makes it possible quickly to "collapse" the determinant $\Delta$ and reduce the whole problem to the graphical determination of several roots of the equation $\Delta = 0$. In this case the exponents of the temporal dependence of the solutions will, generally speaking, be different for different layers and in the general case will be determined by the properties and structure of the entire medium as a whole.

In accordance with the structure of the determinant $\Delta$, the equation $\Delta = 0$ has only simple roots. If these roots are denoted by $s_m$, then, according to (13), by the expansion theorem for images, the solution of equations $(1')$ with boundary conditions $(2')$—$(4')$ can immediately be written in the form

$$U_j(x,t) = c_j + \sum_{m=1}^{\infty} \left\{ \frac{\Delta_{A_j}(s_m)}{\Delta'(s_m)} \operatorname{ch}\left( x\sqrt{\frac{s_m}{D_j}} \right) + \frac{\Delta_{B_j}(s_m)}{\Delta'(s_m)} \operatorname{sh}\left( x\sqrt{\frac{s_m}{D_j}} \right) \right\} e^{s_m t}, \tag{14}$$

whence, by virtue of (5), we finally obtain the solution of the posed problem:

$$u_j(x,t) = c_j e^{-k_j t} + \sum_{m=1}^{\infty} \left\{ \frac{\Delta_{A_j}(s_m)}{\Delta'(s_m)} \operatorname{ch}\left( x\sqrt{\frac{s_m}{D_j}} \right) + \frac{\Delta_{B_j}(s_m)}{\Delta'(s_m)} \operatorname{sh}\left( x\sqrt{\frac{s_m}{D_j}} \right) \right\} e^{(s_m - k_j)t}, \tag{15}$$

where $j = 1, 2, \ldots, n$; $\Delta'(s_m)$ is the value of the derivative $\partial\Delta/\partial s$ at $s = s_m$.

Formula (15) makes it possible to find directly, with any desired degree of accuracy depending only on the accuracy of the graphical determination of the roots of the equation $\Delta = 0$, the final solutions of equations (1). Thus the whole problem is reduced to computing the determinants $\Delta$, $\Delta_{A_j}$, and $\Delta_{B_j}$, and to finding the first several roots of the equation $\Delta = 0$. In comparison with the amount of computational work required in the Green' s-function method or in the method of finite integral transforms, the indicated calculations constitute a very simple operation. At the same time, different variants of specifying the "external" boundary conditions—in the form of prescribed concentrations, fluxes, or surface sources—introduce changes only into the "corner" minors of second order of the determinant $\Delta$, while the entire solution scheme remains practically unchanged.

In contrast to the direct numerical approximate solution of similar problems, the analytic expressions obtained by this method make possible a theoretical analysis of diffusion processes in each of the media under consideration in general form.

**Remark.** If $\Delta_{A_j}$ and $\Delta_{B_j}$ are not entire, but meromorphic functions of $s$, then in formulas (14) and (15) $\Delta_{A_j}$ and $\Delta_{B_j}$ should be understood as the numerators of these functions, and $\Delta'(s)$ as the derivatives of the product of the characteristic determinant $\Delta$ by their denominators.

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*Note: Figure translations are in progress. See original paper for figures.*