Mathematical Modeling and Simulation of Processes of Heterodiffusion with Cascade Decay of Particles

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Математичне та Комп'ютерне Моделювання Процесів Гетеродифузії за Каскадного Розпаду Частинок

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***Abstract*—The mathematical model of mass transfer processes with taken into consideration of a local medium structure and cascade decay of admixture particles migrating in two ways is constructed. For the specific scheme of cascade, the balance relations of mass of the system components are formulated, the linear state equations and kinetic relationships are obtained. The heterodiffusion processes of admixture with its cascade decay in a body with two migration ways, accompanied by mass exchange between states, are investigated. For the case of unramified cascade decay, associated initial-boundary value heterodiffusion problems by cascade kind, when the problem solutions at one stage are sources on the next, are formulated. Solutions of the problems are obtained by iterative procedure with using Green functions. The expressions for diffusion fluxes of migrating admixture substances through the given section of the body and amount of decaying substances that passed through the layer in a certain time interval.**

***Анотація*—Побудована математична модель процесів масоперенесення домішкових речовин з урахуванням локальної структури середовища та каскадного розпаду домішкових частинок, які мігрують двома шляхами. Для конкретної схеми каскадного розпаду сформульовано балансові співвідношення маси компонент системи, отримано лінійні рівняння стану та кінетичні співвідношення. Досліджено процеси гетеродифузії домішок за їх каскадного розпаду в тілі з двома шляхами міграції, що супроводжуються масообміном між станами. Для випадку нерозгалуженого каскадного розпаду сформульовані зв'язані крайові задачі гетеродифузії каскадного типу, коли розв'язки задачі на одному етапі є джерелами на наступному.**

Розв'язки задач побудовані за ітераційною процедурою з використанням функцій Гріна. Отримано формули для дифузійних потоків мігруючих домішкових речовин через заданий переріз тіла та кількості розпадних речовин, що пройшли через шар, за певний часовий інтервал.

Keywords—mathematical model; heterodiffusion; cascade decay; initial-boundary value problems by cascade kind; software; architecture of program complex

Ключові слова—математична модель; гетеродифузія; каскадний розпад; крайова задача каскадного типу; пакет програм; архітектура комплексу програм

I. INTRODUCTION

Mathematical models of admixture heterodiffusion in two ways in media where migrating particles occur locally in different physical states and differ substantially by their mobilities [1-3], are used for describing the processes of mass transfer in polycrystals, fine-grained systems of different nature, porous fluid-saturated media, ets. For example, a significant numbers of metals and allows used in engineering are polycrystals. Their structures are characterized by availability of dislocations, grain boundaries and internal boundaries of interphases [4].

An important feature of the processes of heterodiffusion of technogenic substances is their natural decay (degradation), which occur with the same intensity in each of physically different states. In some cases, the substance generated in the process of decay is already less toxic and its redistribution is not of interest for further study. At the same time the generated substance can decay and generate new substance which migrates in two ways, is sorbed-desorbed and decay. Such a process is called cascade decay and can occur as a result of radioactive decay or chemical reactions (in particular, chain reactions), for example [5]:

$$^{137}Te \longrightarrow {}^{137}I \longrightarrow {}^{137}Xe \longrightarrow {}^{137}Cs \longrightarrow {}^{138}Cs \longrightarrow {}^{138}Ba\ .$$

In the work the mathematical model of heterodiffusion of admixture particles in two ways under their cascade decay is constructed, associated initial-boundary value heterodiffusion problems by cascade kind, when the problem solutions at one stage are sources on the next, are formulated. The solutions of the problems are found and on this basis software is designed.

II. MATHEMATICAL MODEL

A. Object of inquiry

Let decaying particles of one chemical kind migrate in a body with two migration ways and mass exchange between states [1, 3, 6, 7]. Moreover, the substances that formed as a result of decay can also decay. We accept that the body $\mathbf{K}^*$ (discrete set of material particles) is a multicomponent solid solution. We assume interacting discrete sets of material particles $\mathbf{K}_j^{*(0)}$ that form the base of the body ($j=0$) and admixture particles in two dedicated states ($j=1;2$) as thermodynamical components of the system. When the substance $\mathbf{K}_j^{*(0)}$ in the state $j=1;2$ decays, the particles of other substances $\mathbf{K}_j^{*(1)}$ and $\mathbf{K}_j^{*(N)}$ are formed, and the particles $\mathbf{K}_j^{*(N)}$ do not decay yet (fig. 1). In turn, the particles of admixture $\mathbf{K}_j^{*(1)}$ decay and generate the particles of substance $\mathbf{K}_j^{*(2)}$ and non-decaying (harmless) substances, which be attributed to $\mathbf{K}_j^{*(N)}$, and so on, while we obtain only non-decaying admixture substances in the ($N-1$)-th step.

We juxtapose the continuums $\mathbf{K}_j^{(i)}$ ($i=\overline{0,N}$, $j=\overline{0,2}$) to each component of the body (subsets of particles $\mathbf{K}_0^{*(0)}$ that forms the skeleton and to the particles of decaying substance in different states $\mathbf{K}_j^{*(0)}$ as well as the particles that formed as a result of decay $\mathbf{K}_j^{*(i)}$ ($j=1;2$, $i=\overline{1,N}$)).

B. Balance relations

As reference relations of the model we assume the balance equations for masses of each component of the system. If the change in mass of the component occurs due to mass fluxes and internal sources [8], then the equations of balance of mass of the component ij take place

$$\frac{\partial \rho_j^{(i)}}{\partial t} = -\vec{\nabla}\cdot\left(\rho_j^{(i)}\vec{v}_j^{(i)}\right) + w_j^{(i)} \quad (i=\overline{0,N},\ j=\overline{0,2}), \tag{1}$$

where $\rho_j^{(i)}$ are the densities of the system components, $\vec{v}_j^{(i)}$ is the velocities of motion of material points of the continuums $\mathbf{K}_j^{(i)}$; $\vec{\nabla}$ is Hamilton's nabla-operator; $w_j^{(i)}$ is the density of internal source (or sink) of component ij ; the dot is the scalar product [7].

Since we have assumed that the processes of sorption-desorption and decay of admixture are treated as source (sink) of the component, then in the general case the capacity of mass product $w_j^{(i)}$ can be presented as a sum

$$w_j^{(i)} = \sum_{\substack{k=0\\k\neq j}}^{2} \omega_{jk}^{(i)} + \overline{w}_j^{(i)} \quad (i=\overline{0,N},\ j=\overline{0,2}), \tag{2}$$

where $\omega_{jk}^{(i)}$ is the capacity of mass product of the component i in the state j in connection with its transition from the continuum $\mathbf{K}_k^{(i)}$; $\overline{w}_j^{(i)}$ is the capacity of mass product of the component ij due to decay of particles of the component $i-1$ ($i=\overline{1,N}$, $j=1,2$). Then we have

$$\overline{w}_j^{(0)} = 0 \quad (\forall j), \qquad \sum_{j=1}^{2}\sum_{i=1}^{N} \overline{w}_j^{(i)} = 0\ ; \tag{3}$$

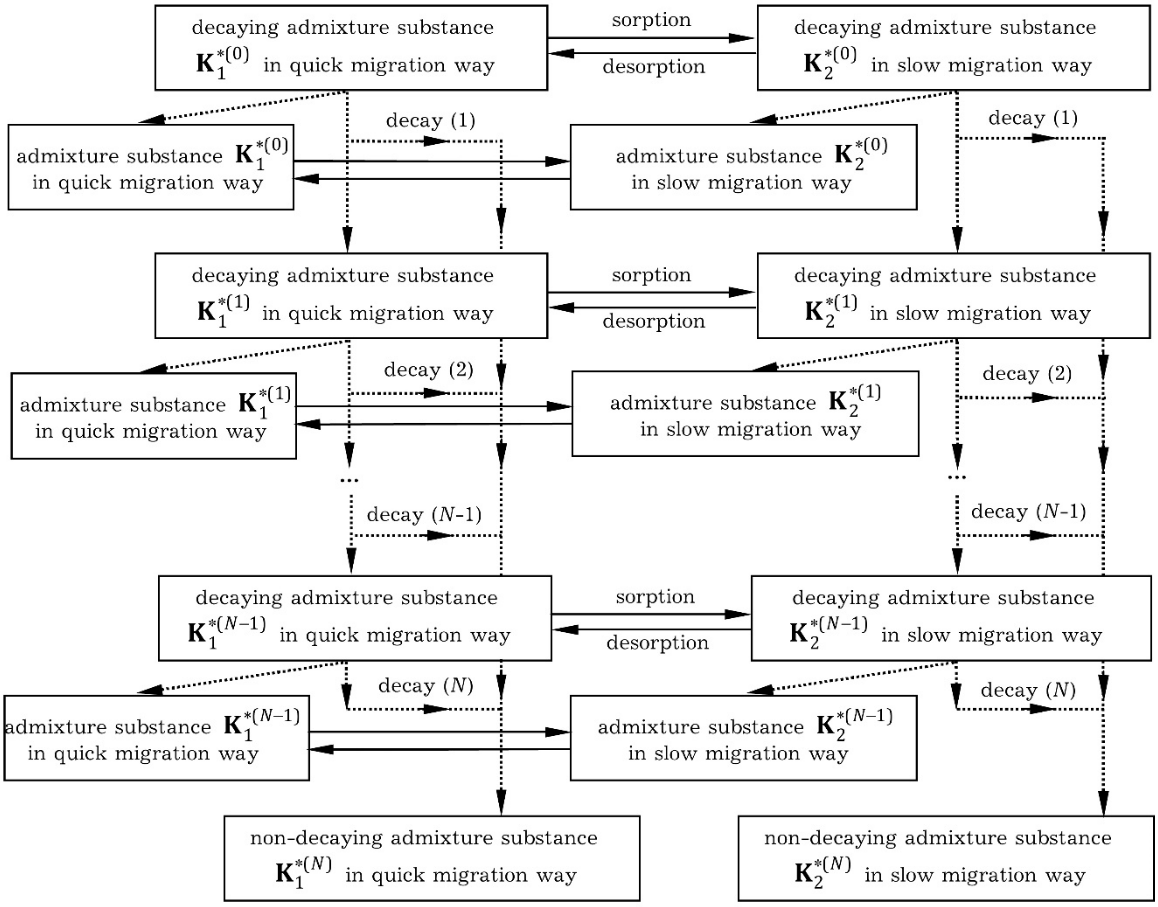

Fig. 1. Scheme of cascade decay of admixture components of the thermodynamic system and sorption-desorption processes

including

$$\omega_{jj}^{(i)}=0 \quad (\forall j),\ \omega_{jk}^{(i)}=-\omega_{kj}^{(i)} \quad (\forall i,j,k),\ \sum_{j=0}^{2}\sum_{k=0}^{2}\omega_{jk}^{(i)}=0\ (\forall i).$$

Let values of the body density $\rho=\sum_{i,j}\rho_j^{(i)}$ and velocity $\vec{v}$ introduced by the following equation

$$\vec{v}=\sum_{j=0}^{2}\sum_{i=0}^{N}\rho_j^{(i)}\vec{v}_j^{(i)}\Big/\rho\,, \qquad (4)$$

is attributed to the points of the continuum of mass centres $\mathbf{K}_c$. We add Eq.(1) by all indexes i and j.

Using the expressions (2) and (4) we obtain

$$\frac{\partial\rho}{\partial t}=-\vec{\nabla}\cdot\rho\sum_{j=0}^{2}\sum_{i=0}^{N}\frac{\rho_j^{(i)}\vec{v}_j^{(i)}}{\rho}=-\rho\vec{\nabla}\cdot\vec{v}-\vec{v}\cdot\vec{\nabla}\rho\,. \qquad (5)$$

Using that the total derivation with respect to time is $\mathrm{d}/\mathrm{d}t=\partial/\partial t+\vec{v}\cdot\vec{\nabla}$, the Eq.(5) can be written as

$$\frac{\mathrm{d}\rho}{\mathrm{d}t}=-\rho\vec{\nabla}\cdot\vec{v}\,. \qquad (6)$$

Write equation of balance for mass of component ij per the total derivative with respect to time

$$\frac{\mathrm{d}\rho_j^{(i)}}{\mathrm{d}t}=\vec{\nabla}\cdot\left(\rho_j^{(i)}\vec{v}\right)-\vec{\nabla}\cdot\left(\rho_j^{(i)}\vec{v}\right)-\rho_j^{(i)}\vec{\nabla}\cdot\vec{v}+w_j^{(i)}$$

Take into account that $\rho_j^{(i)}=C_j^{(i)}\rho$, where $C_j^{(i)}=\rho_j^{(i)}\big/\rho$ is the mass concentration of component satisfying the condition of normalization

$$\sum_{j=0}^{2}\sum_{i=0}^{N}C_j^{(i)}=1\,. \qquad (7)$$

Then we obtain

$$\frac{d\rho_j^{(i)}}{dt}+\rho_j^{(i)}\vec{\nabla}\cdot\vec{v}=\rho\frac{dC_j^{(i)}}{dt}+C_j^{(i)}\frac{d\rho}{dt}+C_j^{(i)}\rho\vec{\nabla}\cdot\vec{v}=\rho\frac{dC_j^{(i)}}{dt},$$

because the relation (6) is valid. As a result we obtain equation of balance of concentration of the component i in the state j

$$\rho\frac{dC_j^{(i)}}{dt}=-\vec{\nabla}\cdot\rho_j^{(i)}\left(\vec{v}_j^{(i)}-\vec{v}\right)+w_j^{(i)}=-\vec{\nabla}\cdot\vec{J}_j^{(i)}+w_j^{(i)}$$

The quantity $\vec{J}_j^{(i)}=\rho_j^{(i)}\left(\vec{v}_j^{(i)}-\vec{v}\right)$ is the diffusion flux of the component ij, introduced with respect to the points of the continuum $\mathbf{K}_c$.

Note that if we use the normalization condition (7), than balance equation can be written as

$$\rho\frac{dC_j^{(i)}}{dt}=-\vec{\nabla}\cdot\vec{J}_j^{(i)}+w_j^{(i)},\quad i=\overline{0,N},\ j=1,2, \tag{8}$$

$$C_0^{(0)}=1-\sum_{j=1}^{2}\sum_{i=0}^{N}C_j^{(i)}. \tag{9}$$

C. Kinetic equations and state equetions

If we have the aggregate of conjugate thermodynamic forces and corresponding thermodynamic fluxes $\vec{X}_j^{(i)}\div\vec{J}_j^{(i)}$, $X_k^{(i)}\div\omega_k^{(i)}$, here the linear kinetic relations are

$$\vec{J}_j^{(i)}=\sum_{m=1}^{2}\sum_{n=0}^{N}L_{jm}^{(in)}\vec{X}_m^{(n)},\quad L_{jm}^{(in)}=\left(\frac{\partial\vec{J}_j^{(i)}}{\partial\vec{X}_m^{(n)}}\right)_0;$$

$$\omega_k^{(i)}=\sum_{m=1}^{2}\sum_{l=1}^{N}\lambda_{km}^{(il)}X_m^{(l)},\quad \lambda_{km}^{(il)}=\left(\frac{\partial\omega_k^{(i)}}{\partial X_m^{(l)}}\right)_0, \tag{10}$$

where $\vec{X}_j^{(i)}$ is vector thermidynamic force conjugated to vector diffusion flux $\vec{J}_j^{(i)}$, namely [7]

$$\vec{X}_j^{(i)}=-\vec{\nabla}\left(\mu_j^{(i)}+\psi_j^{(i)}\right); \tag{11}$$

$X_m^{(l)}$ is thermodynamic force conjugated to thermodynamic flux $\omega_m^{(l)}$; $\mu_j^{(i)}$ is the chemical potential of the component ij, $\psi_j^{(i)}$ is potential energy of mass unit of component i in the state j. So long as $\psi_j^{(0)}=\psi_j^{(1)}=...=\psi_j^{(N)}=\psi$, the taking into account the conditions (3), which the capacities of mass products $w_j^{(i)}$, we obtain

$$\sum_{j=0}^{2}\sum_{i=0}^{N}\psi_j^{(i)}w_j^{(i)}=\psi\sum_{j=0}^{2}\sum_{i=0}^{N}w_j^{(i)}=0.$$

Let us take into account only the processes of transitions of admixture particles between two ways of migration $\omega_{12}^{(i)}$ ($i=\overline{1,N}$), i.e. the capacities of mass products due to the processes of sorption-desorption $\omega_{12}^{(i)}$ and $\omega_{21}^{(i)}$ are non-zero. Thereto, the capacities of mass products $\overline{w}_j^{(i)}$ for the components $i=\overline{1,N}$ obey the conditions

$$\overline{w}_j^{(i)}=\overline{w}_j^{(ii-1)}+\overline{w}_j^{(ii+1)}+\overline{w}_j^{(iN)},\quad \overline{w}_j^{(11)}=0,$$
$$\overline{w}_j^{(i+1i)}=-\overline{w}_j^{(ii+1)}\quad (i=\overline{1,N},\ j=1,2),$$
$$\overline{w}_j^{(ii\pm l)}=0 \text{ for } l\geq 2,\ \overline{w}_j^{(ii)}=0 \text{ for } \forall i;\ \overline{w}_j^{(iN)}=-\overline{w}_j^{(Ni)},$$
$$\overline{w}_j^{(N)}=\sum_{i=1}^{N-1}\overline{w}_j^{(Ni)}=-\sum_{i=1}^{N-1}\overline{w}_j^{(iN)};\ \overline{w}_j^{(i)}=0\ (j=0);$$
$$\overline{w}^{(i)}=\overline{w}_1^{(i)}=\overline{w}_2^{(i)}\ (i=\overline{1,N}).$$

Here $\overline{w}_j^{(ii-1)}$ is the capacities of mass products of substance $\mathbf{K}_j^{(i)}$ in j-th state at the i-th stage of cascade decay due to decay of substance $\mathbf{K}_j^{(i-1)}$; $\overline{w}_j^{(ii+1)}$, $\overline{w}_j^{(iN)}$ are the capacities of mass sink of substance $\mathbf{K}_j^{(i)}$ at the stage $i+1$ and the last stage of decay $i=N$ in the j-th way of migration.

Then we have

$$\sum_{j=1}^{2}\sum_{i=0}^{N}\mu_j^{(i)}w_j^{(i)}=\sum_{j=1}^{2}\sum_{i=0}^{N}\mu_j^{(i)}\left[\sum_{k=1}^{2}\omega_{jk}^{(i)}+\overline{w}_j^{(i)}\right]. \tag{12}$$

The first term of the right-hand side of (12) can be modified to the form

$$\sum_{j=1}^{2}\sum_{i=0}^{N}\sum_{k=1}^{2}\mu_j^{(i)}\omega_{jk}^{(i)}=-\sum_{i=1}^{N}\left(\mu_2^{(i)}-\mu_1^{(i)}\right)\omega_{12}^{(i)}.$$

Denote $\omega_1^{(i)}=\omega_{12}^{(i)}$ ($i=\overline{1,N}$) are the scalar mass flows characterizing mass exchange between states; $X_1^{(i)}$ are the scalar thermodynamic forces conjugated to corresponding mass flows $\omega_j^{(i)}$, namely

$$X_1^{(i)}=\mu_2^{(i)}-\mu_1^{(i)}\ (i=\overline{0,N}). \tag{13}$$

We present the second term of the right-hand side of (12) as

$$\sum_{i=0}^{N}\mu_j^{(i)}\overline{w}_j^{(i)}=-\sum_{i=1}^{N-1}\left(\mu_j^{(i+1)}-\mu_j^{(i)}\right)\overline{w}_j^{(ii+1)}-\sum_{i=1}^{N-1}\left(\mu_j^{(N)}-\mu_j^{(i)}\right)\overline{w}_j^{(iN)},$$

Where we assume that $\overline{w}_j^{(ik)}$, $\overline{w}_j^{(iN)}$ ($i,k=\overline{1,N-1}$) are scalar mass flows characterizing decay of admixture particles and we consider them known; $\overline{X}_j^{(i)} = \mu_j^{(i+1)} - \mu_j^{(i)}$, $\overline{X}_j^{(Ni)} = \mu_j^{(N)} - \mu_j^{(i)}$ ($i = \overline{1,N}$, $j = 1,2$) are scalar quantities conjugated to corresponding mass flows $\overline{w}_j^{(ik)}$, $\overline{w}_j^{(iN)}$.

As a consequence of Onsager's conditions of reciprocity [9], the coefficients $L_{jm}^{(in)}$, $\lambda_{km}^{(il)}$ have to satisfy the conditions $L_{jm}^{(in)} = L_{mj}^{(ni)}$, $\lambda_{km}^{(il)} = \lambda_{mk}^{(li)}$, and due to the second low of thermodynamics they obey such restrictions: $L_{jj}^{(ii)}, \lambda_{kk}^{(ii)} \geq 0$, $L_{jj}^{(ii)} L_{mm}^{(nn)} \geq (L_{jm}^{(in)} + L_{mj}^{(ni)})^2/4$, $\lambda_{kk}^{(ii)} \lambda_{mm}^{(ll)} \geq (\lambda_{km}^{(il)} + \lambda_{mk}^{(li)})^2/4$.

The linear state equations is

$$\mu_j^{(i)} = \mu_{j0}^{(i)} + \sum_{k=1} d_{jk}^{(i)} c_k^{(i)} . \tag{14}$$

Here $\mu_{j0}^{(i)}$ is the chemical potential of pure substance of the component ij; $d_j^{(i)} = \left(\partial \mu_j^{(i)} / \partial c_j^{(i)}\right)_0$ are the material characteristics of the system.

D. Key sets of model equations

As solving functions, we choose the derivation of concentration of admixture components $c_j^{(i)} = C_j^{(i)} - C_j^{(i)0}$ from the values in the reference state $C_j^{(i)0}$, which corresponds with the natural state of unlimited body without external influence.

If we substitute the expressions for thermodynamic forces (11), (13) into kinetic equations for the thermodynamic fluxes (10), then we obtain

$$\vec{J}_j^{(i)} = -\sum_{m=1}^{2} \sum_{n=0}^{N} L_{jm}^{(in)} \vec{\nabla} \mu_m^{(n)}, \quad \omega_k^{(i)} = \sum_{l=0}^{N} \lambda_{k1}^{(il)} \left(\mu_2^{(l)} - \mu_1^{(l)}\right).$$

We express the chemical potentials per solving functions using the linear state equations (14). Accept that the material characteristics are independent on coordinates. Then

$$\vec{J}_j^{(i)} = -\sum_{m=1}^{2} \sum_{n=0}^{N} L_{jm}^{(in)} d_m^{(n)} \vec{\nabla} c_m^{(n)},$$

$$\omega_k^{(i)} = \sum_{l=0}^{N} \left[\overline{\lambda}_{k1}^{(il)} c_1^{(l)} + \overline{\lambda}_{k2}^{(il)} c_2^{(l)} + M_k^{(il)}\right], \tag{15}$$

where $\overline{\lambda}_{k1}^{(il)} = -\lambda_{k1}^{(il)} d_1^{(l)}$, $\overline{\lambda}_{k2}^{(il)} = \left(\lambda_{k1}^{(il)} - \lambda_{k2}^{(il)}\right) d_2^{(l)}$ are the concentrative coefficients of intensity of the processes of intertransition of particles between states; $M_k^{(il)} = -\lambda_{k1}^{(il)} \mu_{10}^{(l)} + \left(\lambda_{k1}^{(il)} - \lambda_{k2}^{(il)}\right) \mu_{20}^{(l)}$ are the model constants.

Sum of terms in the expression (15) of type $\overline{\lambda}_{k1}^{(il)} c_1^{(l)} + \overline{\lambda}_{k2}^{(il)} c_2^{(l)} + M_k^{(il)}$ is describing the mass product of the component of the thermodynamic system. From the beginning we have assumed change of admixture mass can occur only due to particles transitions between states and due to decay of substance. That is $M_k^{(il)} \equiv 0$.

If we substitute the expressions for the thermodynamic fluxes of admixture (15) into equation of balance of components concentration (8), then we obtain the equations of heterodiffusion in the form

for $i = 0$

$$\rho \frac{\mathrm{d} c_1^{(0)}}{\mathrm{d}t} = \vec{\nabla} \cdot \left[\sum_{m=1}^{2} \sum_{n=0}^{N} D_{1m}^{(0n)} \vec{\nabla} c_m^{(n)}\right] + \sum_{l=0}^{N} \left[\overline{\lambda}_{11}^{(0l)} c_1^{(l)} + \overline{\lambda}_{12}^{(0l)} c_2^{(l)}\right] - \widetilde{\widetilde{\lambda}}_1^{(1)} c_1^{(0)} - \widetilde{\lambda}_1^{(0N)} c_1^{(0)},$$

$$\rho \frac{\mathrm{d} c_2^{(0)}}{\mathrm{d}t} = -\vec{\nabla} \cdot \left[\sum_{m=1}^{2} \sum_{n=0}^{N} D_{2m}^{(0n)} \vec{\nabla} c_m^{(n)}\right] - \sum_{l=0}^{N} \left[\overline{\lambda}_{11}^{(0l)} c_1^{(l)} + \overline{\lambda}_{12}^{(0l)} c_2^{(l)}\right] + \sum_{l=0}^{N} \left[\overline{\lambda}_{21}^{(0l)} c_1^{(l)} + \overline{\lambda}_{22}^{(0l)} c_2^{(l)}\right] - \widetilde{\widetilde{\lambda}}_2^{(1)} c_2^{(0)} - \widetilde{\lambda}_2^{(0N)} c_2^{(0)};$$

for $i = \overline{1, N-1}$

$$\rho \frac{\mathrm{d} c_1^{(i)}}{\mathrm{d}t} = \vec{\nabla} \cdot \left[\sum_{m=1}^{2} \sum_{n=0}^{N} D_{1m}^{(in)} \vec{\nabla} c_m^{(n)}\right] + \sum_{l=0}^{N} \left[\overline{\lambda}_{11}^{(il)} c_1^{(l)} + \overline{\lambda}_{12}^{(il)} c_2^{(l)}\right] + \widetilde{\lambda}_1^{(i-1)} c_1^{(i-1)} - \widetilde{\widetilde{\lambda}}_1^{(i+1)} c_1^{(i)} - \widetilde{\lambda}_1^{(iN)} c_1^{(i)},$$

$$\rho \frac{\mathrm{d} c_2^{(i)}}{\mathrm{d}t} = -\vec{\nabla} \cdot \left[\sum_{m=1}^{2} \sum_{n=0}^{N} D_{2m}^{(in)} \vec{\nabla} c_m^{(n)}\right] - \sum_{l=0}^{N} \left[\overline{\lambda}_{11}^{(il)} c_1^{(l)} + \overline{\lambda}_{12}^{(il)} c_2^{(l)}\right] + \sum_{l=0}^{N} \left[\overline{\lambda}_{21}^{(il)} c_1^{(l)} + \overline{\lambda}_{22}^{(il)} c_2^{(l)}\right] + \widetilde{\lambda}_2^{(i-1)} c_2^{(i-1)} - \widetilde{\widetilde{\lambda}}_2^{(i+1)} c_2^{(i)} - \widetilde{\lambda}_2^{(iN)} c_2^{(i)};$$

for $i = N$

$$\rho \frac{\mathrm{d} c_1^{(N)}}{\mathrm{d}t} = \vec{\nabla} \cdot \left[\sum_{m=1}^{2} \sum_{n=0}^{N} D_{1m}^{(Nn)} \vec{\nabla} c_m^{(n)}\right] + \sum_{l=0}^{N} \left[\overline{\lambda}_{11}^{(Nl)} c_1^{(l)} + \overline{\lambda}_{12}^{(Nl)} c_2^{(l)}\right] + \sum_{i=0}^{N-1} \widetilde{\lambda}_1^{(iN)} c_1^{(i)}$$

$$\rho \frac{\mathrm{d} c_2^{(N)}}{\mathrm{d}t} = -\vec{\nabla} \cdot \left[\sum_{m=1}^{2} \sum_{n=0}^{N} D_{2m}^{(Nn)} \vec{\nabla} c_m^{(n)}\right] - \sum_{l=0}^{N} \left[\overline{\lambda}_{11}^{(Nl)} c_1^{(l)} + \overline{\lambda}_{12}^{(Nl)} c_2^{(l)}\right] + \sum_{l=0}^{N} \left[\overline{\lambda}_{21}^{(Nl)} c_1^{(l)} + \overline{\lambda}_{22}^{(Nl)} c_2^{(l)}\right] + \sum_{i=0}^{N-1} \widetilde{\lambda}_2^{(iN)} c_2^{(i)} . \tag{16}$$

Here $D_{jm}^{(in)} = L_{jm}^{(in)} d_m^{(n)}$ are the kinetic coefficients of diffusion; $\widetilde{\lambda}_j^{(i-1)}$, $\widetilde{\widetilde{\lambda}}_j^{(i+1)}$, $\widetilde{\lambda}_j^{(iN)}$ are constants defining the decay process.

Take into consideration that admixture of the same chemical kind decays equally in different states (fig. 1), i.e. $\widetilde{\lambda}^{(i)} = \widetilde{\lambda}_j^{(i)}$, $\widetilde{\widetilde{\lambda}}^{(i+1)} = \widetilde{\widetilde{\lambda}}_j^{(i+1)}$, $\widetilde{\lambda}^{(iN)} = \widetilde{\lambda}_j^{(iN)}$. Also take into account only the processes of diffusion and sorption-desorption of particles of one chemical kind. Also we consider that chemical reactions that led to decay of substance are irreversible. And we assume independence of the model coefficients on coordinates, neglect the convective term, and then the key model of heterodiffusion in two ways under cascade decay of migrating substances (16) takes the form

for $i = 0$

$$\frac{\partial c_1^{(0)}}{\partial t} = \overline{D}_{11}^{(0)} \Delta c_1^{(0)} + \overline{D}_{12}^{(0)} \Delta c_2^{(0)} - \overline{k}_1^{(0)} c_1^{(0)} + \overline{k}_2^{(0)} c_2^{(0)} - \tilde{\tilde{\lambda}}_1^{(1)} c_1^{(0)} - \tilde{\lambda}_1^{(0N)} c_1^{(0)},$$

$$\frac{\partial c_2^{(0)}}{\partial t} = \overline{D}_{21}^{(0)} \Delta c_1^{(0)} + \overline{D}_{22}^{(0)} \Delta c_2^{e(0)} + \overline{k}_1^{(0)} c_1^{(0)} - \overline{k}_2^{(0)} c_2^{(0)} - \tilde{\tilde{\lambda}}_2^{(1)} c_2^{(0)} - \tilde{\lambda}_2^{(0N)} c_2^{(0)};$$

for $i = \overline{1, N-1}$

$$\frac{\partial c_1^{(i)}}{\partial t} = \overline{D}_{11}^{(i)} \Delta c_1^{(i)} + \overline{D}_{12}^{(i)} \Delta c_2^{(i)} - \overline{k}_1^{(i)} c_1^{(i)} + \overline{k}_2^{(i)} c_2^{(i)} + \tilde{\lambda}_1^{(i-1)} c_1^{(i-1)} - \tilde{\tilde{\lambda}}_1^{(i+1)} c_1^{(i)} - \tilde{\lambda}_1^{(iN)} c_1^{(i)},$$

$$\frac{\partial c_2^{(i)}}{\partial t} = \overline{D}_{21}^{(i)} \Delta c_1^{(i)} + \overline{D}_{22}^{(i)} \Delta c_2^{(i)} + \overline{k}_1^{(i)} c_1^{(i)} - \overline{k}_2^{(i)} c_2^{(i)} + \tilde{\lambda}_2^{(i-1)} c_2^{(i-1)} - \tilde{\tilde{\lambda}}_2^{(i+1)} c_2^{(i)} - \tilde{\lambda}_2^{(iN)} c_2^{(i)};$$

for $i = N$

$$\frac{\partial c_1^{(N)}}{\partial t} = \overline{D}_{11}^{(N)} \Delta c_1^{(N)} + \overline{D}_{12}^{(N)} \Delta c_2^{(N)} - \overline{k}_1^{(N)} c_1^{(N)} + \overline{k}_2^{(N)} c_2^{(N)} + \sum_{i=0}^{N-1} \tilde{\lambda}_1^{(iN)} c_1^{(i)},$$

$$\frac{\partial c_2^{(N)}}{\partial t} = \overline{D}_{21}^{(N)} \Delta c_1^{(N)} + \overline{D}_{22}^{(N)} \Delta c_2^{(N)} + \overline{k}_1^{(N)} c_1^{(N)} - \overline{k}_2^{(N)} c_2^{(N)} + \sum_{i=0}^{N-1} \tilde{\lambda}_2^{(iN)} c_2^{(i)}. \qquad (17)$$

Here $\overline{D}_{jm}^{(i)} = D_{jm}^{(ii)} / \rho$ ($j,m = 1,2$, $i = \overline{0,N}$) are the coefficients of diffusion; $\overline{k}_1^{(i)} = -\lambda_{12}^{(ii)} / \rho$, $\overline{k}_2^{(i)} = \lambda_{21}^{(ii)} / \rho$ are the coefficients of intensity of the processes of particles transitions between states.

The sets of heterodiffusion equations (17) need to be supplemented by the equation for finding the concentration of the material particles (8) as well as the equation of continuity (6).

III. Initial-boundary value heterodiffusion problems of cascade kind

For one-dimensional in spatial coordinate case in the natural dimensionless form [10] heterodiffusion in two ways under cascade decay of migration particles is described by the following sets of partial differential equations at different stages of cascade decay:

for $i = 0$

$$\frac{\partial c_1^{(0)}}{\partial \tau} = \frac{\partial^2 c_1^{(0)}}{\partial \xi^2} + d_1^{(0)} \frac{\partial^2 c_2^{(0)}}{\partial \xi^2} - a_{11}^{(0)} c_1^{(0)} + a_{12}^{(0)} c_2^{(0)},$$

$$\frac{\partial c_2^{(0)}}{\partial \tau} = d_2^{(0)} \frac{\partial^2 c_1^{(0)}}{\partial \xi^2} + d^{(0)} \frac{\partial^2 c_2^{(0)}}{\partial \xi^2} + a_{21}^{(0)} c_1^{(0)} - a_{22}^{(0)} c_2^{(0)}; \qquad (18a)$$

for $i = \overline{1, N-1}$

$$\frac{\partial c_1^{(i)}}{\partial \tau} = d_0^{(i)} \frac{\partial^2 c_1^{(i)}}{\partial \xi^2} + d_1^{(i)} \frac{\partial^2 c_2^{(i)}}{\partial \xi^2} - a_{11}^{(i)} c_1^{(i)} + a_{12}^{(i)} c_2^{(i)} + a_{\lambda 1}^{(i-1)} c_1^{(i-1)},$$

$$\frac{\partial c_2^{(i)}}{\partial \tau} = d_2^{(i)} \frac{\partial^2 c_1^{(i)}}{\partial \xi^2} + d^{(i)} \frac{\partial^2 c_2^{(i)}}{\partial \xi^2} + a_{21}^{(i)} c_1^{(i)} - a_{22}^{(i)} c_2^{(i)} + a_{\lambda 2}^{(i-1)} c_2^{(i-1)}; \qquad (18b)$$

for $i = N$

$$\frac{\partial c_1^{(N)}}{\partial \tau} = d_0^{(N)} \frac{\partial^2 c_1^{(N)}}{\partial \xi^2} + d_1^{(N)} \frac{\partial^2 c_2^{(N)}}{\partial \xi^2} - a_{11}^{(N)} c_1^{(N)} + a_{12}^{(N)} c_2^{(N)} + \sum_{i=0}^{N-1} a_{\lambda 1}^{(iN)} c_1^{(i)},$$

$$\frac{\partial c_2^{(N)}}{\partial \tau} = d_2^{(N)} \frac{\partial^2 c_1^{(N)}}{\partial \xi^2} + d^{(N)} \frac{\partial^2 c_2^{(N)}}{\partial \xi^2} + a_{21}^{(N)} c_1^{(N)} - a_{22}^{(N)} c_2^{(N)} + \sum_{i=0}^{N-1} a_{\lambda 2}^{(iN)} c_2^{(i)}, \qquad (18)$$

where $d_0^{(i)}$, $d^{(i)}$ are the reduced coefficients of diffusion of substance $\mathbf{K}_j^{(i)}$ ($i = \overline{0,N}$) at i-th step of decay in states $j = 1$ and 2, $d_1^{(i)}$, $d_2^{(i)}$ are the reduced crossed coefficients of diffusion [7]; $a_{11}^{(i)} = \left(k_1^{(i)} + \tilde{\lambda}_1^{(i+1)} + \lambda_1^{(iN)}\right) / k_2^{(0)}$, $a_{22}^{(i)} = \left(k_2^{(i)} + k_3^{(i)} + \tilde{\lambda}_2^{(i+1)} + \lambda_2^{(iN)}\right) / k_2^{(0)}$, $a_{12}^{(i)} = k_2^{(i)} / k_2^{(0)}$, $a_{21}^{(i)} = k_1^{(i)} / k_2^{(0)}$; $a_{\lambda j}^{(i-1)} = \lambda_j^{(i-1)} / k_2^{(0)}$ is the coefficient of intensity of decay of $\mathbf{K}_j^{(i-1)}$ ($i = \overline{1,N}$, $j = 1;\ 2$), $a_{\lambda 1}^{(iN)}$ is the coefficient determining part of non-decaying substance that has been generated through decay at the i-th step $\mathbf{K}_j^{(i)}$ ($i = \overline{0, N-1}$, $j = 1;\ 2$); $k_1^{(i)}$, $k_2^{(i)}$ are the coefficients of intensity of the processes of transitions between states; $\lambda_j^{(i-1)}$, $\tilde{\lambda}_j^{(i+1)}$, $\lambda_j^{(iN)}$ are the constants determining the decay process.

In sets of equations (18a)-(18c) we have used the dimensionless variables $\tau = k_2^{(0)} t$; $\xi = \left(k_2^{(0)} / D_{11}^{(0)}\right)^{1/2} x$, where t is time, x is the spatial coordinate; $k_2^{(0)}$ is the coefficient of intensity of transitions of particles of $\mathbf{K}^{(0)}$ from the second state into the first one at zero stage of decay; $D_{11}^{(0)}$ is the coefficient of diffusion of substance $\mathbf{K}_1^{(0)}$ in quick migration way $j = 1$. Further consider $d_0^{(i)} < d_1^{(i)}$, $i = \overline{1,N}$, $d_0^{(0)} = 1$.

Assume that at the initial moment admixtures were absent in the body, namely

$$c_1^{(i)}(\xi, \tau)\Big|_{\tau=0} = c_2^{(i)}(\xi, \tau)\Big|_{\tau=0} = 0, \quad i = \overline{0,N}, \qquad (19)$$

for $\tau > 0$ on the body surface $\xi = 0$ it is kept the constant value of total concentration c_0 of substance $\mathbf{K}^{(0)}$, which is distributed among different migration ways for $i=0$ as follows

$$c_1^{(0)}(\xi,\tau)\Big|_{\xi=0}=\alpha c_0\,,\quad c_2^{(0)}(\xi,\tau)\Big|_{\xi=0}=(1-\alpha)c_0\,,\qquad (20a)$$

where α ($0\le\alpha\le 1$) is the parameter determining the part of admixture that came from the body surface into the quick way.

For $i=1,...,N$ we assume zero boundary condition at the top layer surface:

$$c_1^{(i)}(\xi,\tau)\Big|_{\xi=0}=0\,,\quad c_2^{(i)}(\xi,\tau)\Big|_{\xi=0}=0\,,\qquad i=\overline{1,N}\,.\quad (20b)$$

We assume that the particles concentrations at all stages of decay equal zero at "bottom" boundary of the body, i.e.

$$c_1^{(i)}(\xi,\tau)\Big|_{\xi=\xi_0}=c_2^{(i)}(\xi,\tau)\Big|_{\xi=\xi_0}=0\,,\qquad i=\overline{0,N}\,.\qquad (20c)$$

At zero stage of decay the solutions of heterodiffusion equations (18a) with initial (19) and boundary (20a), (20b) conditions are found using integral transformation. Then we obtain *concentration of decaying admixture in quick migration way*

$$\frac{c_1^{(0)}(\tau,\xi)}{c_0}=\left\{\alpha-\frac{\widetilde{b}_1}{ce}\right\}\left(1-\frac{\xi}{\xi_0}\right)-B\left[\left(\widetilde{a}_1+\frac{\widetilde{b}_1}{x_1}\right)\frac{\sin(\pi-y)x_1}{\sin\pi x_1}-\right.$$
$$\left.-\left(\widetilde{a}_1+\frac{\widetilde{b}_1}{x_2}\right)\frac{\sin(\pi-y)x_2}{\sin\pi x_2}\right]-\frac{2}{\xi_0}\sum_{n=1}^{\infty}\frac{\sin y_n\xi}{y_n(s_1-s_2)}\times$$
$$\times\left[\left(\alpha s_1+p_1+\frac{p_2}{s_1}\right)e^{s_1\tau}-\left(\alpha s_2+p_1+\frac{p_2}{s_2}\right)e^{s_2\tau}\right],\qquad (21a)$$

concentration of decaying admixture in slow migration way

$$\frac{c_2^{(0)}(\tau,\xi)}{c_0}=\left\{1-\alpha-\frac{\widetilde{b}_2}{ce}\right\}\left(1-\frac{\xi}{\xi_0}\right)-B\left[\left(\widetilde{a}_2+\frac{\widetilde{b}_2}{x_1}\right)\frac{\sin(\pi-y)x_1}{\sin\pi x_1}-\right.$$
$$\left.-\left(\widetilde{a}_2+\frac{\widetilde{b}_2}{x_2}\right)\frac{\sin(\pi-y)x_2}{\sin\pi x_2}\right]-\frac{2}{\xi_0}\sum_{n=1}^{\infty}\frac{\sin y_n\xi}{y_n(s_1-s_2)}\times$$
$$\times\left[\left((1-\alpha)s_1+p_1'+\frac{p_2'}{s_1}\right)e^{s_1\tau}-\left((1-\alpha)s_2+p_1'+\frac{p_2'}{s_2}\right)e^{s_2\tau}\right],\ (21b)$$

total concentration of decaying substance $c^{(0)}=c_1^{(0)}+c_2^{(0)}$

$$\frac{c^{(0)}(\tau,\xi)}{c_0}=\left\{1-\frac{\widetilde{b}}{ce}\right\}\left(1-\frac{\xi}{\xi_0}\right)-B\left[\left(\widetilde{a}+\frac{\widetilde{b}}{x_1}\right)\frac{\sin(\pi-y)x_1}{\sin\pi x_1}-\right.$$
$$\left.\left(\widetilde{a}+\frac{\widetilde{b}}{x_2}\right)\frac{\sin(\pi-y)x_2}{\sin\pi x_2}\right]-\frac{2}{\xi_0}\sum_{n=1}^{\infty}\frac{\sin y_n\xi}{y_n(s_1-s_2)}\times$$
$$\times\left[\left(s_1+\widetilde{p}_1+\frac{\widetilde{p}_2}{s_1}\right)e^{s_1\tau}-\left(s_2+\widetilde{p}_1+\frac{\widetilde{p}_2}{s_2}\right)e^{s_2\tau}\right],\qquad (21c)$$

where $B=\dfrac{1}{\sqrt{d^2-4ec^2}}$, $x_{1,2}=\dfrac{1}{2}\left(-\dfrac{d}{c}\pm\sqrt{\dfrac{d^2}{c^2}-4e}\right)$, $\widetilde{a}=\widetilde{a}_1+\widetilde{a}_2$, $\widetilde{b}=\widetilde{b}_1+\widetilde{b}_2$, $\widetilde{p}_l=p_l+p_l'$ ($l=1,2$), $\widetilde{a}_1=\left(d_1^{(0)}\alpha_2+d^{(0)}\alpha_1\right)\dfrac{\pi^2}{\xi_0^2}$, $\widetilde{b}_1=\alpha_1a_{22}^{(0)}-\alpha_2a_{12}^{(0)}$, $\widetilde{a}_2=\dfrac{\pi^2}{\xi_0^2}\left(\alpha_2+\alpha_1d_2^{(0)}\right)$, $\widetilde{b}_2=\alpha_2a_{11}^{(0)}-\alpha_1a_{21}^{(0)}$,

$c=\left(d^{(0)}-d_1^{(0)}d_2^{(0)}\right)\dfrac{\pi^4}{\xi_0^4}$, $e=a_{11}^{(0)}a_{22}^{(0)}-a_{12}^{(0)}a_{21}^{(0)}$,

$d=a_{22}^{(0)}+a_{11}^{(0)}d^{(0)}+ \quad +d_1^{(0)}a_{21}^{(0)}+d_2^{(0)}a_{12}^{(0)}\Big)\dfrac{\pi^2}{\xi_0^2}$

$s_{1,2}=-\eta_1/2\pm\sqrt{(\eta_1/2)^2-\eta_2}$, $\eta_1= \quad =y_n\left(d^{(0)}+1\right)+a_{22}^{(0)}+a_{11}^{(0)}$;
$\eta_2=\left(d^{(0)}-d_1^{(0)}d_2^{(0)}\right)y_n^4+\left(a_{22}^{(0)}+a_{11}^{(0)}d_2^{(0)}+ \quad +d_1^{(0)}a_{21}^{(0)}+d_2^{(0)}a_{12}^{(0)}\right)y_n^2+$
$a_{11}^{(0)}a_{22}^{(0)}-a_{12}^{(0)}a_{21}^{(0)}$; $p_1=(\alpha d^{(0)}-d_1^{(0)}\times$
$\times(1-\alpha))y_n^2+\alpha a_{22}^{(0)}+\alpha_1+(1-\alpha)a_{12}^{(0)}$,
$p_2=\left(d_1^{(0)}\alpha_2+d^{(0)}\alpha_1\right)y_n^2+ \quad +\alpha_1a_{22}^{(0)}-\alpha_2a_{12}^{(0)}$,
$p_1'=\left(1-\alpha-\alpha d_2^{(0)}\right)y_n^2+a(1-\alpha)_{11}^{(0)}+\alpha a_{21}^{(0)}+ \quad +\alpha_2$;
$p_2'=\left(\alpha_2+\alpha_1d_2^{(0)}\right)y_n^2+\alpha_2a_{11}^{(0)}-\alpha_1a_{21}^{(0)}$, $y=\pi\xi/\xi_0$.

Note that for the model of heterodiffusion of decaying substance the asymptotic summand of the obtained solutions are essentially non-linear and consist of various combinations of relation of type $\sin((\pi-y)x)/\sin\pi x$. With that each of such relations is less than 1. Also note that the linear parts of the asymptotic summands of analogical problem heterodiffusion of non-decaying substance, i.e. $1-\xi/\xi_0$, are proportional to the coefficient determining the part of admixture that came from the boundary into the corresponding migration way (α, $1-\alpha$ and 1). At the same time taking into consideration decay of migrating substance leads to the appearance of certain "allowance" in such coefficients ($\widetilde{b}_1/ce$, $\widetilde{b}_2/ce$ and $\widetilde{b}/ce$). Take into account that these "allowances" are nonnegative then linear parts of asymptotes of function (4) are not larger the similar terms of concentrations of non-decaying substances, and in each state separately.

For the other stages of cascade decay $i=\overline{1,N-1}$ solutions of the initial-boundary value problems are presented per corresponding Green functions, considering admixture decay at the previous stage of cascade as mass source at the step i:

$$c_j^{(i)}(\xi,\tau)=a_{\lambda j}^{(i-1)}\int_0^{\tau}\int_0^{\xi_0}G_j^{(i)}\left(\xi,\xi';\tau,\tau'\right)c_j^{(i-1)}\left(\xi',\tau'\right)d\xi'd\tau',\ j=\overline{1;\,2.},(22)$$

Here $G_j^{(i)}(\tau,\tau';\xi,\xi')$ are Green functions of the problems (18b), (19), (20b), (20c) for $i=\overline{1,N-1}$.

For the case of $i=N$ (non-decaying admixture) the process of heterodiffusion is described by the initial-boundary value problem (18c), (19), (20b) and (20c). Its solutions is also presented in terms of Green functions by analogue of the formula (22) for $i=\overline{1,N-1}$, namely

$$c_j^{(N)}(\xi,\tau)=\int_0^{\tau}\int_0^{\xi_0}G_j^{(N)}(\xi,\xi';\tau,\tau')\sum_{i=0}^{N-1}a_{\lambda j}^{(iN)}c_j^{(i)}(\xi',\tau')d\xi'd\tau' \,,\quad j=1,2\,, \tag{23}$$

where $G_j^{(N)}(\xi,\xi';\tau,\tau')$ ($j=1,2$) are Green functions of the problem (18c), (19), (20b) and (20c).

Consequently determination of concentrations at each stage $i=0,...,N-1$ by the formulae (21) and (22) with account expressions for Green functions we find concentrations of non-decaying particles under cascade decay of admixtures.

The analytical form of the obtained concentrations allows au to find expressions for the mass fluxes of decaying substances at different stages of cascade decay through the surface $\xi=\xi_*$, where $0\le\xi_*\le\xi_0$. Proceeding from the linear kinetic relations [11], mass fluxes are determined in the natural dimensionless variables such as

$$J_{*1}^{(i)}(\tau)=-\sqrt{k_2^{(0)}D_{11}^{(0)}}\left[d_0^{(i)}\frac{\partial c_1^{(i)}(\xi,\tau)}{\partial\xi}+d_1^{(i)}\frac{\partial c_2^{e(i)}(\xi,\tau)}{\partial\xi}\right]\Bigg|_{\xi=\xi_*},$$

$$J_{*2}^{(i)}(\tau)=-\sqrt{k_2^{(0)}D_{11}^{(0)}}\left[d_2^{(i)}\frac{\partial c_1^{(i)}(\xi,\tau)}{\partial\xi}+d^{(i)}\frac{\partial c_2^{(i)}(\xi,\tau)}{\partial\xi}\right]\Bigg|_{\xi=\xi_*},\ i=\overline{0;N} \tag{24}$$

and the total flux through the surface $\xi=\xi_*$

$$J_*^{(i)}(\tau)=J_{*1}^{(i)}\Big|_{\xi=\xi_*}+J_{*2}^{(i)}\Big|_{\xi=\xi_*}. \tag{25}$$

If we have obtained the diffusion fluxes of decaying substances then we can find the function [10]

$$Q_0^{(i)}=\int_0^{\tau_*}J_0^{(i)}(\tau)d\tau\,,\quad i=\overline{0,N}\,, \tag{26}$$

which determines quantities of decaying substances $Q_0^{(i)}(\tau)$, that passed through the surface $\xi=\xi_0$ (the bottom body boundary) over time-interval $[0;\tau_*]$.

IV. Architecture of Program Complex for Heterodiffusion Model

On the basis of the formulae (21), (22), (23) for admixture concentrations and corresponding formulae for mass fluxes (24), (25) and quantities of decaying and non-decaying admixture components that passed through the bottom layer surface (26), software has been designed for simulation of mass transfer processes in a body with two migration way that been accompanied sorption-desorption processes and cascade decay of admixtures particles. Architecture of the program complex for simulating mass transfer processes under cascade decay of particles for the model of heterodiffusion in two ways is presented in Fig.2.

Schemes of application modules for calculation of diffusion fluxes and quantity of substances passed through the layer are shown in Figs.3 and 4.

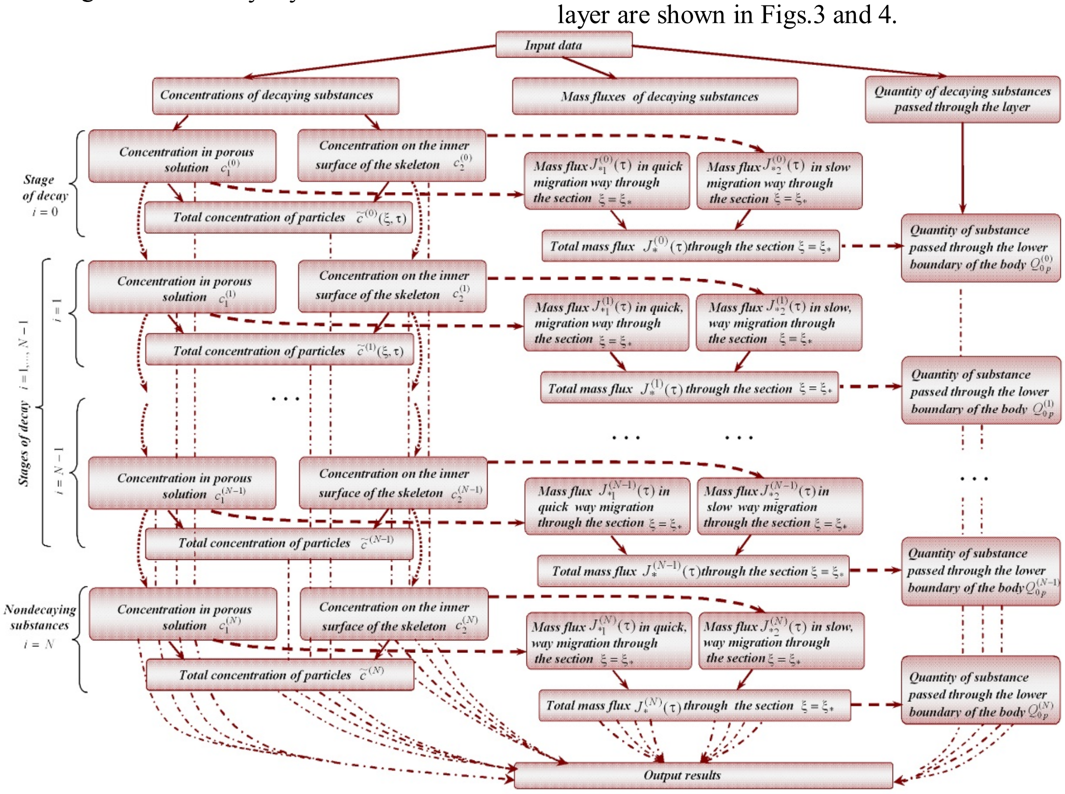

Fig. 2. Architecture of program complex for the model of heterodiffusion in two ways under cascade decay of particles

Fig. 3. Scheme of algorithm of the program module for calculating the diffusion fluxes of decaying substances

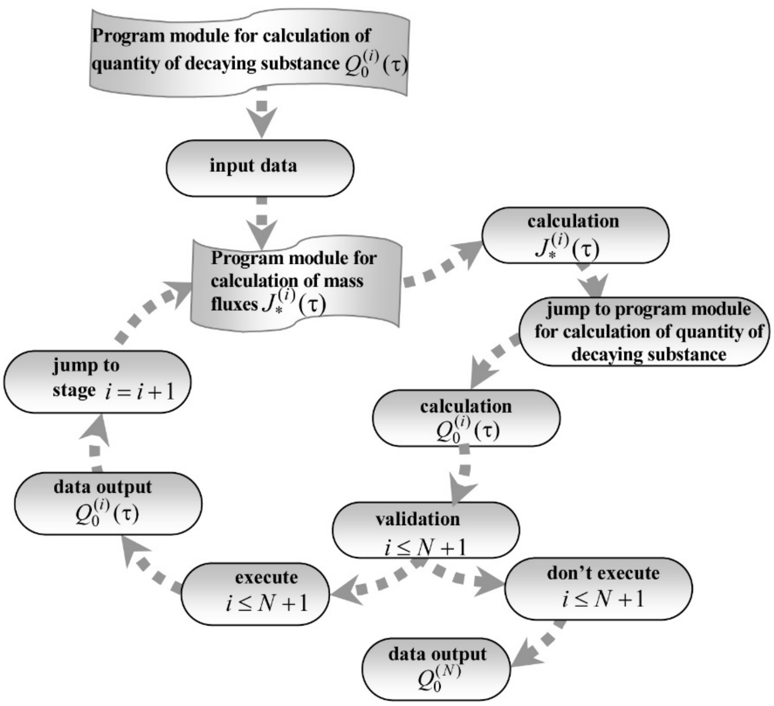

Fig. 4. Scheme of algorithm of the program module for calculating the quantity of decaying substances that passed through the lower boundary of the layer at a given time interval

Note that program modules for fluxes and quantities substances consist of one by one cyclic process, and at each stage the modules interact with the module for concentrations at the previous stage. At the same time the module for calculation of the admixture concentrations contains two cyclic processes.

CONCLUSIONS

Thus, for the description of processes of admixtures mass transfer in two ways under their cascade decay, the mathematical model is constructed where the concentration of particles at certain stage of decay is the mass source of decaying substance diffusing at the next step. For specific scheme of cascade decay the balance relaions for mass of components of the system are formulated. The linear state equations and kinetic relations are obtained. The conditions under which the mass production capacities for the components of the system obey, are established. The key sets of equations of the model of heterodiffusion in two ways under cascade decay of migrating particles are obtained taking into consideration only processes of diffusion and sorption-desorption and under the assumption thhat chemical reactions that led to the decay of substance is irreversible.

On the basis of the constructed model new statements of initial-boundary value problems of cascade type where the concentration of particles at certain step of decay is the mass source of decaying substance at the next, which also diffuses, is sorbed, desorbed and decays. For linear chemical reactions the solutions of the initial-boundary value problems of cascade type are constructed by iterrative procedure with using Green functions. This make it possible to obtain the fluxes of migrating conponents and quantities of corresponding substances that passed through certain substance, for example bottom boundary of the body, for given time interval.

The program package for simulation of mass transfer in the body with two migration ways under cascade decay of admuxtures is designed. Numerical analysis of concentrations of decaying particles and mass fluxes is carried out.

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