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Sensitivity analysis of solutions of two-dimensional admixture heterodiffusion problems with respect to perturbation of medium parameters

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In this paper the sensitivity analysis of solutions of the problems of heterodiffusion of admixture in two-dimensional multiphase media with respect to perturbation of medium parameters is considered. Based on a semi-discrete Galerkin approximation and the finite element method the initial-boundary value problem is reduced to the initial value problem for a system of ordinary differential equations concerning node values of the admixture concentration. The equations of sensitivity in differential, variational and finite-element formulations are obtained. The results of some numerical experiments for heterodiffusion of admixture (pollutant) in a layer of soil which occupied rectangular domain in case of thermodynamic equilibrium among state of admixture in water adsorbed on soil skeleton and in soil skeleton are presented. The influence of small changes of model parameters on distribution of the admixture concentration is analyzed.

Keywords: sensitivity analysis, direct differentiation method, heterodiffusion, two-dimensional multiphase medium, Galerkin semidiscrete approximation, finite element method.

Introduction. During the research of complex systems it is important to investigate the changing effect of various system parameters in regards to the system response. In broad sense sensitivity analysis (SA) consists in calculation of relative changes of output characteristic of the system which is the result of small change of system parameters. As a result of SA, the derivatives of the system characteristic with respect to system parameters (i.e., sensitivity coefficients) are obtained. SA is an essential tool for gradient-based optimization method for solving optimal control problems. Several methods are available for response sensitivity computation, including the finite difference method (FDM), the adjoint method (AM), and the direct differentiation method (DDM). These methods can be derived in continuous and discrete formulation. Different aspects of SA methods can be found in e.g., Haug et al. [1], Marchuk [2], Keulen et al. [3], Choi and Kim [4], Harashchenko and Shvets [5], Peter and Dwight [6]. SA is now recognized as an integral part of the modelling process.

In this paper the SA is used for evaluation of the solution sensitivity of admixture heterodiffusion problems with respect to perturbation of medium parameters. Mass transfer of admixture in nonhomogeneous multiphase media (heterodiffusive process) is modeled by system of parabolic equations. Constitutive relationships of the model for heterodiffusion in two ways with traps in one of them were first developed by Chaplia and Chernukha [7]. Based on analytical representation of the solution (usually in form of trigonometric series) Chaplia and Chernukha [8] have obtained numerical results for set of heterodiffusive processes in one- and two-dimensional multiphase media. Note, that with using analytical approach some difficulties can be faced when characteristics of media vary with time and space; and also in the case of irregular shape of region. Application of numerical methods makes it possible to find out the solution in these cases. Shcherbata [9] applied variational approach and FEM for solving of one-dimensional heterodiffusion problems with variable with time and space characteristics of media. Savula and Shcherbata [10] applied FDM and DDM in continuous and discrete formulation for SA of solutions of one-dimensional heterodiffusion problem with respect to perturbation of medium parameters. In this paper FDM and DDM are developed for SA of solutions of two-dimensional heterodiffusion problem.

1. Mathematical model of heterodiffusive process

Consider a multiphase medium (for example, a layer of soil) in domain Ω_x with boundary Γ_x, $\bar{\Omega}_x = \Omega_x \cup \Gamma_x$, $x = (x_1, x_2) \in \bar{\Omega}_x$, $\bar{\Omega}_x \in R^2$. Suppose that physically small volume element of waterlogged medium (solid solution) contains parts of admixture, which can be in three different phases of media: in water, in adsorbed water on soil skeleton and in soil skeleton.

Denote $\mathbf{c}(x,t) = [c_1(x,t), ..., c_m(x,t)]^{\mathrm{T}}$ the concentration of admixture (pollutant) at the point of medium x at time t, $t \in \Omega_t = (t_0, t_e]$, where m is the number of the phase of medium, in which admixture is contained. Concentration $\mathbf{c}(x,t)$ is composed by the concentration of admixture in different phases (in water, in adsorbed water on soil skeleton and in soil skeleton). In the case of invariable total density of medium, the heterodiffusive process of admixture is modeled by the system of partial differential equations of parabolic type, proposed by Chaplia and Chernukha [7]

$$\frac{\partial c_i}{\partial t} = \nabla \cdot \left(\sum_{j=1}^{m} D_{ij} \nabla c_j \right) + \sum_{j=1}^{m} k_{ij} c_j + f_i, \quad (x,t) \in \Omega = \Omega_x \times \Omega_t, \; i = \overline{1,m}, \tag{1}$$

where $f_i(x,t)$, $i = \overline{1,m}$ are the intensity of internal sources of pollutant, D_{ij}, $i, j = \overline{1,m}$ are diffusion coefficients and k_{ij}, $i, j = \overline{1,m}$ are coefficients of rate of transition of admixture from one phase to other. Here is used the following notation of the operator $\nabla : \nabla g(x) = \mathrm{grad}(g(x))$, $\nabla \cdot \mathbf{r}(x) = \mathrm{div}(\mathbf{r}(x))$; $g(x)$, $\mathbf{r}(x)$ are scalar and vector functions of spatial coordinates respectively.

Equations (1) are added with the initial condition

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$$c_i\left(x,t_0\right)=c_{0i}(x), \qquad i=\overline{1,m}, \quad x\in\bar{\Omega}_x, \tag{2}$$

and boundary conditions

$$\mathbf{n}\cdot\left(\sum_{j=1}^{m}D_{ij}\nabla c_j\right)+\sum_{j=1}^{m}\alpha_{ij}(x,t)c_j=\beta_i(x,t), \quad (x,t)\in\Gamma, \;\; \Gamma=\Gamma_x\times\Omega_t, \;\; i=\overline{1,m}, \tag{3}$$

where **n** is the outward unit normal.

In general, three different phases of the medium ($m = 3$) can contain admixture. Note that in the case of thermodynamic equilibrium among state of admixture in different phases, it is possible to define effective total concentrations. Therefore, the mathematical model (1)-(3) of heterodiffusive process can consist of two ($m = 2$) or even one ($m = 1$) equation, see Chaplia and Chernukha [7].

Solution $\mathbf{c}(x,t)$ depends on the value of coefficients of equations (1)-(3). Let denote a vector of coefficients of diffusion and mass transfer as $\mathbf{u}=\left[\mathbf{u}_D^T,\mathbf{u}_K^T\right]^{\mathrm{T}}=\left[u_1,\dots,u_{\tilde{p}}\right]^{\mathrm{T}}$, $\mathbf{u}_D=\left[u_{D1},\dots,u_{Dp_1}\right]^T=\left[D_{11},\dots,D_{mm}\right]^{\mathrm{T}}$, $\mathbf{u}_K=\left[u_{K1},\dots,u_{Kp_2}\right]^T=\left[k_{11},\dots,k_{mm}\right]^{\mathrm{T}}$, $\tilde{p}=p_1+p_2$. The influence of the proposed above vector on the solution $\mathbf{c}(x,t)$ has been analyzed through this paper. To emphasize the dependency of any variable on **u**, let point to such variable with subscript **u**.

Let us create the following matrices and vectors

$$\mathbf{D}=\left[D_{ij}\right]_{i,j=1}^{m}, \quad \mathbf{K}=\left[k_{ij}\right]_{i,j=1}^{m}, \quad \nabla\mathbf{c}=\left[\nabla c_1,\dots,\nabla c_m\right]^{\mathrm{T}},$$

$$\mathbf{L_u c}=\boldsymbol{\Lambda}_\mathbf{u}\mathbf{c}+\mathbf{Kc}, \; \boldsymbol{\Lambda}_\mathbf{u}\mathbf{c}=\left[\Lambda_{1\mathbf{u}},\dots,\Lambda_{m\mathbf{u}}\right]^{\mathrm{T}}, \; \Lambda_{i\mathbf{u}}=\nabla\cdot\left(\sum_{j=1}^{m}D_{ij}\nabla c_j\right)+\sum_{j=1}^{m}k_{ij}c_j, \; i=\overline{1,m},$$

$$\mathbf{f}=\left[f_1,\dots,f_m\right]^{\mathrm{T}}, \quad \mathbf{c}_0=\left[c_{01},..,c_{0m}\right]^{\mathrm{T}}, \quad \boldsymbol{\alpha}=\left[\alpha_{ij}\right]_{i,j=1}^{m}, \quad \boldsymbol{\beta}=\left[\beta_1,\dots,\beta_m\right]^{\mathrm{T}},$$

$$\mathbf{B_u c}=\left[B_{1\mathbf{u}},\dots,B_{m\mathbf{u}}\right]^{\mathrm{T}}, \quad B_{i\mathbf{u}}=\mathbf{n}\cdot\left(\sum_{j=1}^{m}D_{ij}\nabla c_j\right)+\sum_{j=1}^{m}\alpha_{ij}(x,t)c_j, \quad i=\overline{1,m}.$$

Taking into account introduced above matrices and vectors, the initial-boundary value problem (IBVP) (1)-(3) can be written in matrix form

$$\frac{\partial\mathbf{c}}{\partial t}=\mathbf{L_u c}+\mathbf{f}, \qquad (x,t)\in\Omega, \tag{4}$$

$$\mathbf{c}\left(x,t_0\right)=\mathbf{c}_0, \qquad x\in\bar{\Omega}_x, \tag{5}$$

$$\mathbf{B_u c}=\boldsymbol{\beta}, \quad (x,t)\in\Gamma. \tag{6}$$

2. Variational formulation of the problem. Galerkin semidiscrete approximation and finite element method (FEM)

Let us define the following spaces of functions

$$\mathbf{V}_0 = \left\{ \mathbf{v}(x) = \left[v_1(x),\dots,v_m(x) \right]^{\mathrm{T}} : \quad v_i(x) \in W_2^1\left(\Omega_x\right), \quad i = \overline{1,m} \right\},$$
$$\mathbf{V} = \left\{ \mathbf{v}(x,t) = \left[v_1(x,t),\dots,v_m(x,t) \right]^{\mathrm{T}} : \quad v_i(x,t) \in L_2\left(\Omega_t;\mathbf{V}_0\right), \quad i = \overline{1,m} \right\}.$$

Based on variational approach for solving initial-boundary value problems described by Savula [11], Zienkiewicz et al. [12], the IBVP (4)-(6) can be written in variational form: find the function $\mathbf{c} \in \mathbf{V}$, which satisfies the variational equations

$$m\left(\frac{\partial \mathbf{c}}{\partial t}, \mathbf{v}\right) + a_{\mathbf{u}}(\mathbf{c},\mathbf{v}) = l(\mathbf{v}) \qquad \forall \mathbf{v} \in \mathbf{V}_0, \tag{7}$$

$$m\left(\mathbf{c}\left(x,t_0\right) - \mathbf{c}_0(x), \mathbf{v}\right) = 0. \tag{8}$$

Proper bilinear and linear forms can be written as following

$$a_{\mathbf{u}}(\mathbf{c},\mathbf{v}) = \int\limits_{\Omega_x} \left(\mathbf{D}\nabla\mathbf{c}\right)^{\mathrm{T}} \nabla\mathbf{v}\, d\Omega - \int\limits_{\Omega_x} \left(\mathbf{K}\mathbf{c}\right)^{\mathrm{T}} \mathbf{v}\, d\Omega + \int\limits_{\Gamma} \left(\boldsymbol{\alpha}\mathbf{c}\right)^{\mathrm{T}} \mathbf{v}\, d\Gamma,$$
$$m(\mathbf{c},\mathbf{v}) = \int\limits_{\Omega_x} \mathbf{c}^{\mathrm{T}} \mathbf{v}\, d\Omega, \quad l(\mathbf{v}) = \int\limits_{\Omega_x} \mathbf{f}^{\mathrm{T}} \mathbf{v}\, d\Omega + \int\limits_{\Gamma} \boldsymbol{\beta}^{\mathrm{T}} \mathbf{v}\, d\Gamma.$$

To evaluate an approximate solution of the variational problem (7), (8), apply Galerkin discretization procedure and finite element method. Let us choose a sequence of finite dimensional subspaces $\mathbf{V}_n \in \mathbf{V}$ with basis $\boldsymbol{\varphi}_1(x) = \left[\varphi_{11}(x),\dots,\varphi_{1m}(x)\right]^{\mathrm{T}}$,..., $\boldsymbol{\varphi}_n(x) = \left[\varphi_{n1}(x),\dots,\varphi_{nm}(x)\right]^{\mathrm{T}}$ in space of feasible functions $\mathbf{V}$.

Expand the solution of the problem (7), (8) in the same basis $\mathbf{V}_n$

$$\mathbf{c}(x,t) \approx \tilde{\mathbf{c}}(x,t) = \sum_{j=1}^{n} \tilde{\boldsymbol{\varphi}}_j(x) \tilde{\mathbf{C}}_j(t), \tag{9}$$

where $\tilde{\mathbf{C}}_j(t) = \left[C_{j1}(t),\dots,C_{jm}(t)\right]^{\mathrm{T}}$, $C_{ji}(t) \in C^{(1)}\left(\Omega_t\right)$, $j = \overline{1,n}$, $i = \overline{1,m}$ are unknown functions of time coordinate, $\tilde{\boldsymbol{\varphi}}_j(x)$ is matrix composed of basis functions φ_{ji}, $i = \overline{1,m}$, $\tilde{\boldsymbol{\varphi}}_j(x) = \operatorname{diag}\left[\varphi_{j1},\dots,\varphi_{jm}\right]$.

Domain Ω_x is approximated with a union of triangles. As basis functions continuous piecewise linear functions are selected, see Savula [11], Zienkiewicz et al. [12].

Following the Galerkin method, let us substitute $\mathbf{c}$ in equations (7), (8) with the approximate solution (9), and instead of $\mathbf{v}$ put sequentially basic functions $\tilde{\boldsymbol{\varphi}}_j$, $j = \overline{1,n}$.

As result we obtain initial value problem for ordinary differential equations (ODE) in regards to vector-function $\tilde{\mathbf{C}}(t)$

$$\mathbf{M}\frac{\partial\tilde{\mathbf{C}}(t)}{\partial t}+\mathbf{A_u}\tilde{\mathbf{C}}(t)=\mathbf{F}(t), \qquad t\in\Omega_t, \tag{10}$$

$$\mathbf{M}\tilde{\mathbf{C}}(t_0)=\mathbf{P}. \tag{11}$$

The unknown vector-function $\tilde{\mathbf{C}}(t)$ contains the values of the approximate solution $\tilde{\mathbf{C}}_j(t)$, $j=\overline{1,n}$ at the mesh points. The matrices $\mathbf{A_u}$, **M** and vectors **F**, **P** are assembled of the matrices and vectors of finite elements. In matrix notation, we have to solve the linear, large and sparse ODE system. Crank-Nicholson scheme is used to solve problem (10)-(11), see Savula [11], Zienkiewicz et al. [12].

3. Sensitivity analysis

Let us derive the sensitivity of the solution $\mathbf{c}(x,t)$ with respect to change of elements of matrices **D** and **K**. The solution $\mathbf{c}(x,t)$ sensitivity of the governing equation can be obtained by FDMs and DDMs. Overall finite difference consists of repeated execution of the analysis code and the use of a finite difference formula to obtain the derivative. Forward or backward differences are the most popular, see Keulen et al. [3]. However, FDM is high costly because the IBVP must be computed for two or more values of each parameter. Note that finite difference derivatives can suffer from truncation errors with large step size and also from errors when the step size is too small.

The DDMs solve the governing equations of considered process for the sensitivities. The sensitivity equations are obtained by differentiation (discrete or continuous) of the governing equation. In this study, sensitivity equations are obtained in differential, variational and finite-element forms.

3.1. Sensitivity analysis for the initial-boundary value problem. Let us increment (variation) vector **u** with $\delta\mathbf{u}$, $\mathbf{u}^{(1)}=\mathbf{u}+\delta\mathbf{u}$. Matrices **D** and **K** get the increment $\delta\mathbf{D}$ and $\delta\mathbf{K}$ respectively, $\mathbf{D}^{(1)}=\mathbf{D}+\delta\mathbf{D}$, $\mathbf{K}^{(1)}=\mathbf{K}+\delta\mathbf{K}$. Define first-order variations of the solution $\mathbf{c}(x,t)$, operator of governing equations $\mathbf{L_u}$ and operator of boundary conditions $\mathbf{B_u}$ in direction $\delta\mathbf{u}$ based on definition of directional derivative

$$\delta\mathbf{c}=\mathbf{c}'_{\mathbf{u}}\delta\mathbf{u}\equiv\left.\frac{d\mathbf{c}(x,t,\mathbf{u}+\tau\delta\mathbf{u})}{d\tau}\right|_{\tau=0}, \quad \mathbf{c}'_{\mathbf{u}}=\left(\mathbf{c}'_{u_1},\ldots,\mathbf{c}'_{u_{\tilde{p}}}\right)=\left(\frac{\partial\mathbf{c}}{\partial u_1},\ldots,\frac{\partial\mathbf{c}}{\partial u_{\tilde{p}}}\right),$$

$$\mathbf{L}'_{\delta\mathbf{u}}\mathbf{c}=\mathbf{L}'_{\mathbf{u}}\mathbf{c}\delta\mathbf{u}\equiv\left.\frac{d\mathbf{L}_{\mathbf{u}+\tau\delta\mathbf{u}}\mathbf{c}}{d\tau}\right|_{\tau=0}, \quad \mathbf{B}'_{\delta\mathbf{u}}\mathbf{c}=\mathbf{B}'\mathbf{c}\delta\mathbf{u}\equiv\left.\frac{d\mathbf{B}_{\mathbf{u}+\tau\delta\mathbf{u}}\mathbf{c}}{d\tau}\right|_{\tau=0}.$$

Matrices of derivative $\mathbf{L}'_{\mathbf{u}}\mathbf{c}$, $\mathbf{B}'\mathbf{c}$ consist of $\tilde{p}$ columns. Each of them is derived by differentiation of operators $\mathbf{L_u}$, $\mathbf{B_u}$ with respect to component u_p, $p=\overline{1,\tilde{p}}$ of model parameters vector **u**

$$\mathbf{L}'_{\mathbf{u}}\mathbf{c}=\left(\mathbf{L}'_{u_1}\mathbf{c},...,\mathbf{L}'_{u_{\tilde{p}}}\mathbf{c}\right),\quad \mathbf{L}'_{u_p}\mathbf{c}=\begin{cases}\boldsymbol{\Lambda}'_{u_p}\mathbf{c}, & p=\overline{1,p_1},\\ \dfrac{\partial\mathbf{K}}{\partial u_p}\mathbf{c}, & p=\overline{p_1+1,\tilde{p}},\end{cases}$$

$$\boldsymbol{\Lambda}'_{u_p}\mathbf{c}=\left[\Lambda'_{1u_p}\mathbf{c},...,\Lambda'_{mu_p}\mathbf{c},\right],\quad \Lambda'_{iu_p}\mathbf{c}=\nabla\cdot\left(\sum_{j=1}^{m}\frac{\partial D_{ij}}{\partial u_p}\nabla c_j\right),\quad m=\overline{1,m},\quad p=\overline{1,p_1},$$

$$B'_{\mathbf{u}}\mathbf{c}=\left(\mathbf{B}'_{u_1}\mathbf{c},...,\mathbf{B}'_{u_{\tilde{p}}}\mathbf{c}\right),\quad \mathbf{B}'_{u_p}\mathbf{c}=\left[B'_{1u_p}\mathbf{c},...,B'_{mu_p}\mathbf{c}\right],$$

$$B'_{iu_p}\mathbf{c}=\begin{cases}\mathbf{n}\cdot\left(\displaystyle\sum_{j=1}^{3}\frac{\partial D_{ij}}{\partial u_p}\nabla c_j\right), & p=\overline{1,p_1},\\ \mathbf{0}, & p=\overline{p_1+1,\tilde{p}},\end{cases}\qquad i=\overline{1,m}.$$

As a result of differentiation of the equation (4), initial condition (5) and boundary condition (6) with respect to vector **u**, we obtain the following initial-boundary value problem for each of column $\mathbf{c}'_{u_p}$, $p=\overline{1,\tilde{p}}$ of derivative matrix $\mathbf{c}'_{\mathbf{u}}$

$$\frac{\partial\mathbf{c}'_{u_p}}{\partial t}=\mathbf{L_u}\mathbf{c}'_{u_p}+\mathbf{L}'_{u_p}\mathbf{c},\quad (x,t)\in\Omega=\Omega_x\times\Omega_t, \tag{12}$$

$$\mathbf{c}'_{u_p}(x,t_0)=\mathbf{0},\qquad x\in\Omega_x, \tag{13}$$

$$\mathbf{B_u}\mathbf{c}'_{u_p}=-\mathbf{B}'_{u_p}\mathbf{c},\qquad (x,t)\in\Gamma. \tag{14}$$

Problems (12)-(14) have the same structure as original problem (4)-(6). Therefore for solving them we can apply developed variational method and FEM.

3.2. Variational formulation of sensitivity analysis problem. Variational sensitivity equations can be derived by formally differentiation of the variation governing equations (7)-(8) with respect to vector **u**, interchanging the order of the differentiation and using the change rule. As result we obtain the following variational equations for sensitivity vectors $\mathbf{c}'_{u_p}$, $p=\overline{1,\tilde{p}}$

$$m\left(\frac{\partial\mathbf{c}'_{u_p}}{\partial t},\mathbf{v}\right)+a_{\mathbf{u}}\left(\mathbf{c}'_{u_p},\mathbf{v}\right)=-a'_{u_p}(\mathbf{c},\mathbf{v})\qquad \forall\mathbf{v}\in\mathbf{V}_0, \tag{15}$$

$$a'_{u_p}(\mathbf{c},\mathbf{v})=\int_{x_0}^{x_e}\left(\frac{\partial\mathbf{D}}{\partial u_p}\nabla\mathbf{c}\right)^{\mathrm{T}}\nabla\mathbf{v}dx-\int_{x_0}^{x_e}\left(\frac{\partial\mathbf{K}}{\partial u_p}\mathbf{c}\right)^{\mathrm{T}}\mathbf{v}dx,\quad m\left(\mathbf{c}'_{u_p}(x,t_0),\mathbf{v}\right)=\mathbf{0}. \tag{16}$$

Sensitivity equations (12)-(14) i (15), (16) are derived according to continuum approach. Sensitivity equations (15), (16) can be solved by the same FEM that is used for solving original variational problem (7), (8).

3.3. Finite element response sensitivity analysis. In the case of discrete approach, sensitivity equations are derived by differentiation of finite element equations (10), (11). Denote $\tilde{\mathbf{C}}'_{\mathbf{u}}$ derivative matrix of node admixture concentration $\tilde{\mathbf{C}}$ with respect to parameters vector $\mathbf{u}$. As result of differentiation of the equations (10), (11) with respect to $\mathbf{u}$ we derived for sensitivity matrix the following initial problem $\tilde{\mathbf{C}}'_{\mathbf{u}}$ for matrix ordinary differential equation

$$\mathbf{M}\frac{\partial \tilde{\mathbf{C}}'_{\mathbf{u}}(t)}{\partial t}+\mathbf{A}_{\mathbf{u}}\tilde{\mathbf{C}}'_{\mathbf{u}}(t)=-\frac{d\mathbf{A}_{\mathbf{u}}}{d\mathbf{u}}\tilde{\mathbf{C}}(t), \qquad t\in\Omega_t, \tag{17}$$

$$\mathbf{M}\tilde{\mathbf{C}}'_{\mathbf{u}}\left(t_0\right)=\mathbf{0}. \tag{18}$$

Matrix of derivates $\tilde{\mathbf{C}}'_{\mathbf{u}}$ consists of p columns (p is the length of the vector $\mathbf{u}$)

$$\tilde{\mathbf{C}}'_{\mathbf{u}}=\left[\tilde{\mathbf{C}}'_{u_1},\ldots,\tilde{\mathbf{C}}'_{u_{\tilde{p}}}\right]=\left[\frac{\partial\tilde{\mathbf{C}}}{\partial u_1},\ldots,\frac{\partial\tilde{\mathbf{C}}}{\partial u_{\tilde{p}}}\right].$$

Sensitivity matrices $\tilde{\mathbf{C}}'_{\mathbf{u}}$ are evaluated as result of solution of initial value problem for each of columns

$$\mathbf{M}\frac{\partial \tilde{\mathbf{C}}'_{u_p}(t)}{\partial t}+\mathbf{A}_{\mathbf{u}}\tilde{\mathbf{C}}'_{u_p}(t)=-\frac{\partial\mathbf{A}_{\mathbf{u}}}{\partial u_p}\tilde{\mathbf{C}}(t), \qquad p=\overline{1,\tilde{p}}, \quad t\in\Omega_t, \tag{19}$$

$$\mathbf{M}\tilde{\mathbf{C}}'_{u_p}\left(t_0\right)=\mathbf{0}. \tag{20}$$

Matrices of derivates are $\partial\mathbf{A}_{\mathbf{u}}/\partial u_p$ are assembled of the matrices derivates of finite elements. Note that sensitivity equations (19)-(20) can be obtain as a result of application of FEM to variational equations (15), (16). However, continuum SA approach gives an opportunity to substantiate the existence of the derivative $\mathbf{c}'_{\mathbf{u}}$. Apart from that, for solving of continuum sensitivity equations other methods can be applied, which differ from those applied for solving the original problem.

4. Numerical results

In this section we present results of some numerical experiments of hederodiffusion of admixture (pollutant) in a layer of soil which occupies rectangular domain. Assume that thermodynamic equilibrium among state of admixture in water adsorbed on soil skeleton and in soil skeleton exists. In this case, a number of governing equations (1)-(3) is equal to two (m = 2), see Chaplia and Chernukha [7].

As proposed in above mentioned work, let convert governing equations (1)-(3) to dimensionless form using substitution of variables $\tau = k_2 t,\ \xi_i = \left(k_2/D_1\right)^{1/2} x_i,\ i = 1,2$, $\xi = \left(\xi_1, \xi_2\right)$. As a result of such replacement, domain Ω_x, boundary Γ_x and Ω_t are transformed to Ω_ξ, Γ_ξ and $\Omega_\tau = \left(\tau_0, \tau_e\right]$ respectively. Matrices **D** and **K** take the following forms

$$\mathbf{D} = \begin{bmatrix} 1 & d_1 \\ d_2 & d \end{bmatrix}, \qquad \mathbf{K} = \begin{bmatrix} -a & 1 \\ a & -1 \end{bmatrix}.$$

Denote diffusion and mass transfer coefficients as a vector $\mathbf{u} = \left[d, d_1, d_2, a\right]^{\mathrm{T}}$. We research the sensitivity of concentrations c_1, c_2 with respect to these coefficients. Assume that diffusion coefficients and mass transfer coefficients are constants in a domain over the period of time Ω_τ.

Let present the boundary Γ_ξ as a union of tree parts, $\Gamma_\xi = \bigcup_{i=1}^{3} \Gamma_{i\xi}$, $\Gamma_{1\xi} = [BC]$, $\Gamma_{2\xi} = (AB] \cup (CD]$, $\Gamma_{2\xi} = (DE) \cup [EF] \cup (FA)$, Fig. 1. Define boundary condition in the following form

$$c_1\left(\xi,\tau\right) = \alpha c_s,\quad c_2\left(\xi,\tau\right) = (1-\alpha) c_s,\quad \xi \in \Gamma_{1\xi},$$
$$c_1\left(\xi,\tau\right) = 0,\qquad c_2\left(\xi,\tau\right) = 0,\qquad \xi \in \Gamma_{2\xi},$$
$$\frac{\partial c_1}{\partial \mathbf{n}} = 0,\qquad \frac{\partial c_2}{\partial \mathbf{n}} = 0,\qquad \xi \in \Gamma_{3\xi}.$$

Permanent source of admixture is located on the boundary $\Gamma_{1\xi}$. It means that on $\Gamma_{1\xi}$ there is defined the total concentration c_s: $c_1\left(\xi,\tau\right) = \alpha c_s$, $c_2\left(\xi,\tau\right) = (1-\alpha) c_s$. Parameter α $(0 \le \alpha \le 1)$ defines a part of admixture, which penetrates from surface of soil into water and is adsorbed on soil skeleton. There is no admixture on the other upper surface $\Gamma_{2\xi}$ of soil. On the surface of the boundary $\Gamma_{3\xi}$, the mass isolation boundary conditions are specified. The are no internal sources of pollutant in soil, $f_i\left(\xi,\tau\right) = 0,\ i = 1,2$, $(\xi,\tau) \in \Omega_\xi \times \Omega_\tau$. At the initial time τ_0, contentions of admixture equal zero: $c_i\left(\xi,\tau_0\right) = 0,\ i = 1,2$.

We present the result of numerical simulation for the following values of model parameters: $d = 0{,}1$; $d_1 = 0{,}05$; $d_2 = 0{,}05$; $a = 10$; $A(0, 0)$; $B(2, 0)$; $C(4, 0)$; $D(6, 0)$; $E(6, -10)$; $F(-10, 0)$; $c_s = 1$; $\tau_0 = 0$; $\tau_e = 1000$; $\alpha = 1$.

Distribution of total concentration $C\left(\xi,\tau_e\right) = c_1\left(\xi,\tau_e\right) + c_2\left(\xi,\tau_e\right)$ of admixture at time τ_e is shown in Fig. 2. The concentration of admixture is increasing in small part inside of the domain close to source of admixture (boundary $\Gamma_{1\xi}$) and slightly variable in other part of domain.

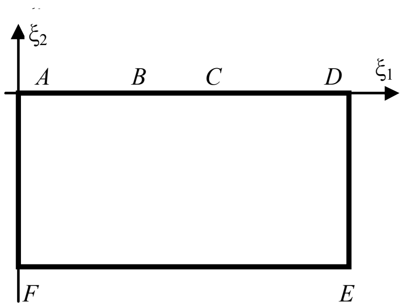

Fig. 1. Layer of soil of rectangular shape

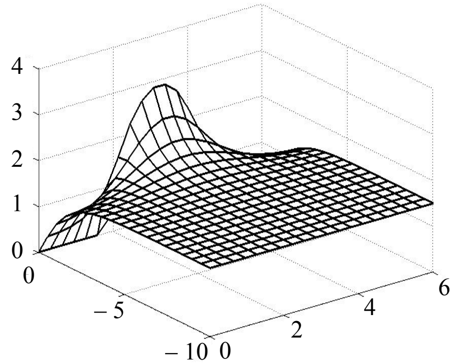

Fig. 2: Distribution of total concentration C of admixture at time τ_e

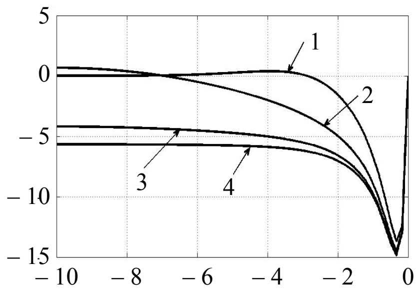

Fig. 3. Sensitivity $\partial C/\partial d$ in section $\xi_1 = 3$ at different point of time

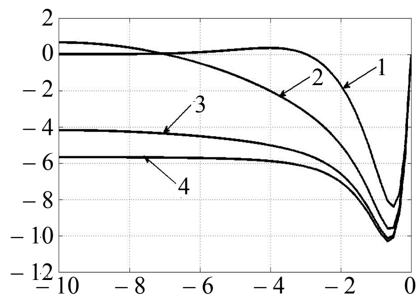

Fig. 4. Sensitivity $\partial C/\partial d_1$ in section $\xi_1 = 3$ at different point of time

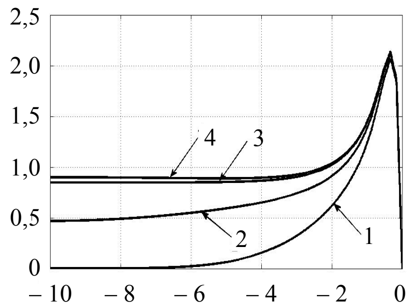

Fig. 5. Sensitivity $\partial C/\partial d_2$ in section $\xi_1 = 3$ at different point of time

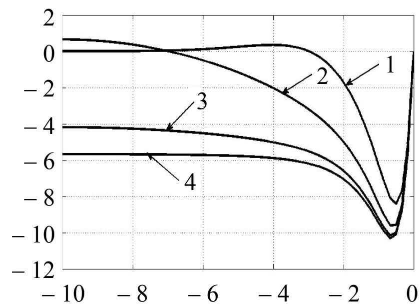

Fig. 6. Sensitivity $\partial C/\partial a$ in section $\xi_1 = 3$ at different point of time

Figures 3-6 show distribution of sensitivity of total concentration $\partial C/\partial u_i = \partial c_1/\partial u_i + +\partial c_2/\partial u_i$, $i = \overline{1,4}$ in section $\xi_1 = 3$ at different points of time. Curves 1-4 display sensitivity $\partial C/\partial u_i$ at points of time $\tau = 10$, $\tau = 100$, $\tau = 500$, $\tau = 1000$.

Thus, as we expected, absolute values of the concentration sensitivity with respect to different model parameters increase in time and achieve steady state. Figures 3-6 show that the increase of parameters' values d, d_1 lead to the decrease of total concentration C. Increasing parameters' values d_2, a lead to decreasing of total concentration C. Similar effects of small changes of model parameters on distribution of the admixture concentration were obtained by Savula and Shcherbata [10] for one-dimensional heterodiffusion problem.

Conclusions. The sensitivity analysis of solutions of the problems of heterodiffusion of admixture in two-dimensional bodies with respect to perturbation of medium parameters is considered. Based on a semi-discrete Galerkin approximation and the finite element method, the initial-boundary value problem is reduced to the initial value problem for a system of ordinary differential equations concerning node values of the admixture concentration. Based on FDM and DDM, the equations of sensitivity in differential, variational and finite-element formulations are obtained. The results of numerical experiments for a layer of soil of rectangular shape are presented and the influence of small changes of model parameters on distribution of the admixture concentration is analyzed.

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Аналіз чутливості розв'язків задач двовимірної гетеродифузії домішкової речовини стосовно змін параметрів середовища

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У цій роботі розглянуто чутливість розв'язків задач гетеродифузії домішкової речовини в двовимірних тілах стосовно малих змін параметрів середовища. Із використанням напівдискретних апроксимацій Гальоркіна та методу скінченних елементів початково-крайову задачу гетеродифузії зведено до задачі Коші для системи звичайних диференціальних рівнянь щодо вузлових значень концентрацій домішки. Отримано рівняння чутливості в диференціальному, варіаційному та скінченно-елемементному формулюваннях. Наведені результати числових експериментів для задач гетеродифузії домішкової речовини (забруднювача) у шарі ґрунту, який займає прямокутну область, для випадку термодинамічної рівноваги між шаром води, адсорбованої на скелеті ґрунту, та скелетом ґрунту. Проаналізовано вплив малих змін параметрів моделі на розподіл концентрації домішкової речовини.

Анализ чувствительности решений задач двумерной гетеродиффузии примесного вещества относительно изменений параметров среды

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В данной работе рассмотрено чувствительность решений задач гетеродиффузии примесного вещества в двумерных телах относительно изменениям параметров среды. С использованием полудискретных аппроксимаций Галёркина и метода конечных элементов начально-краевую задачу гетеродиффузии сведено к задаче Коши для системы обыкновенных дифференциальных уравнений относительно узловых значений концентраций примеси. Получены уравнения чувствительности в дифференциальной, вариационной и конечно-элементной постановках. Приведены результаты численных экспериментов для задач гетеродиффузии примесного вещества в слое почвы, занимающей прямоугольную область, для случая термодинамического равновесия между слоем воды, адсорбированном на скелете почвы, и скелетом почвы. Проанализировано влияние малых изменений параметров модели на распределение концентраций примесного вещества.

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