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The Mathematical Modeling of Metals Mass Transfer in Three Layer Peat Blocks

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Abstract. **The mathematical model for calculation of concentration of metals for 3 layers peat blocks is developed due to solving the 3-D boundary-value problem in multilayered domain – averaging and finite difference methods are considered. As an example, mathematical models for calculation of Fe and Ca concentrations have been analyzed.**

Keywords**: averaging method, finite difference method, boundary conditions of third type, heavy metals, peat bog.**

I INTRODUCTION

Being based on the experimental data the mathematical model for calculation of concentration of metals in different points for different 3 layers (peat blocks) is developed.

An averaging [3] and finite difference method by solving the 3-D boundary-value problem with boundary conditions of the 3rd type in the N-layered domain of homogeneous materials with piece-wise diffusion coefficients, the concentrations functions in every layer and the fixed source function are in question.

The boundary-value problem herein deals with solving the elliptic type of second order for the partial differential equation with piece-wise diffusion coefficients in the N-layered domain.

Similarly, the results of a number of the previously modeled diffusion processes without mass transfer showed a comparatively good compatibility with the experimental data [1].

By using the averaging method with quadratic splines developed by A. Buikis [3], a finite-difference scheme was created. In its turn, it was used to reduce a 3-D boundary-value problem to a system of 2-D partial differential equations, which simplifies the task considerably.

II MATERIALS AND METHODS

1. A mathematical model

The process of diffusion the metal in the peats block is consider in 3-D parallelepiped

$$\Omega = \{(x, y, z): 0 \le x \le l, 0 \le y \le L, 0 \le z \le Z\}$$

The domain - consist of multilauer medium. We will consider the stationary 3-D problem of the linear diffusion theory for multilayered piece-wise homogenous materials of *N* layers in the form

$$\Omega_i = \{(x, y, z): x \in (0, l), y \in (0L), z \in (z_{i-1}, z_i)\}, i = \overline{1, N}$$

where $H_i = z_i - z_{i-1}$ is the height of layer Ω_i, $z_0 = 0$, $z_N = Z$. We will find the distribution of concentrations $c_i = c_i(x, y, z)$ in every layer Ω_i at the point $(x, y, z) \in \Omega_i$ by solving the following partial differential equation (PDE):

$$D_{ix}\partial^2 c_i / \partial x^2 + D_{iy}\partial^2 c_i / \partial y^2 + D_{iz}\partial^2 c_i / \partial z^2 + f_i(x, y, z) = 0 \quad (1.1)$$

where D_{ix}, D_{iy}, D_{iz} are constant diffusions coefficients, $c_i = c_i(x, y, z)$ - the concentrations functions in every layer, $f_i(x, y, z)$ - the fixed sours function. The values c_i and the flux functions $D_{iz}\partial c_i / \partial z$ must be continues on the contact lines between the layers $z = z_i, i = \overline{1, N-1}$:

$$c_i\big|_{z_i} = c_{i+1}\big|_{z_i},\ D_{iz}\partial c_i / \partial z\big|_{z_i} = D_{(i+1)z}\partial c_{i+1} / \partial z\big|_{z_i},\ i = \overline{1, N-1} \quad (1.2)$$

where $i = \overline{1, N-1}$.

We assume that the layered material is bounded above and below with the plane surfaces $z_0 = 0, z = Z$ with fixed boundary conditions in following form:

$$c_N(x, y, Z) = C_a(x, y) \quad (1.3)$$

where $C_0(x, y)$, $C_a(x, y)$ are given concentration-functions, α is the mass transfer coefficient.

We have two forms of fixed boundary conditions in the x, y directions:

1) the periodical conditions by $x = 0,\ x = l$ in the form

$$c_i(0,y,z) = c_i(l,y,z),\ \partial c_i(0,y,z)/\partial x = \partial c_i(l,y,z)/\partial x \quad (1.4)$$

2) the symetrical conditions by $y = 0,\ y = L$

$$\partial c_i(x,0,z)/\partial y = \partial c_i(x,L,z)/\partial y = 0 \quad (1.5)$$

For solving the problem (1.1)-(1.5) we will consider conservative averaging (AV) and finite difference (FD) methods. These procedures allow to reduce the 3-D problem to some 2D boundary value problem for the system of partial differential equations with circular matrix in the x - directions.

2. The AV–method with quadratic splines

The equation of (1.1) is averaged along the heights H_i of layers Ω_i and quadratic integral splines along z coordinate in following form one used [2]:

$$c_i(x,y,z) = C_i(x,y) + m_i(x,y)(z-\bar{z}_i) + \\ + e_i(x,y)G_i\left((z-\bar{z}_i)^2/H_i^2 - 1/12\right) \quad (2.1)$$

where $G_i = H_i/D_{iz}$, $\bar{z}_i = (z_{i-1}+z_i)/2$, m_i, e_i, C_i are the unknown coefficients of the spline-function, $C_i(x,y) = H_i^{-1}\int_{z_{i-1}}^{z_i} c_i(x,y,z)dz$ are the average values of c_i, $i = \overline{1,N}$.

After averaging the system (1.1) along every layer Ω_i, we obtain system of N equations of 2-D PDE

$$D_{ix}\partial^2 C_i/\partial x^2 + D_{iy}\partial^2 C_i/\partial y^2 + 2H_i^{-1}e_i + F_i(x,y) = 0 \quad (2.2)$$

where $F_i = H_i^{-1}\int_{z_{i-1}}^{z_i} f_i(x,y,z)dz$ are the average values of f_i, $i = \overline{1,N}$.

From boundary conditions (1.3) follows

$$\frac{6}{\alpha}(D_{1z}m_1 - e_1) + 3m_1H_1 = 6(C_1 - C_0) + e_1G_1,$$
$$3m_NH_N = 6(C_a - C_N) - e_NG_N$$

From (1.2) follows

$$3m_i + e_iG_i = 6(C_{i+1} - C_i) - 3H_{i+1}m_{i+1} + e_{i+1}G_{i+1},$$
$$D_{iz}m_i + e_i = D_{(i+1)z}m_{i+1} - e_{i+1},\quad i = \overline{1,N-1} \quad (2.4)$$

From (2.1), (2.3), (2.4) we obtain following system of $N-2$ algebraic equations for determining e_i

$$2e_{i-1}G_{i-1}(G_i+G_{i+1}) + e_i\left((G_i+3G_{i-1})(G_i+G_{i+1}) + (G_i+3G_{i+1})(G_i+G_{i-1})\right) + \\ + 2e_{i+1}G_{i+1}(G_i+G_{i-1}) = 6(C_{i+1}-C_i)(G_i+G_{i-1}) - 6(C_i-C_{i-1})(G_i+G_{i+1}) \quad (2.5)$$

and for determining e_1, e_N

$$e_1\left(2G_1 + 4G_2 + \frac{2}{\alpha}\left(4 + \frac{6G_2}{G_1}\right)\right) + 2e_2\left(G_2 + \frac{2G_2}{\alpha G_1}\right) = 6(C_2 - C_1)\left(1 - \frac{2}{\alpha G_1}\right) \\ - 6(C_1 - C_0)\left(1 + \frac{G_2}{G_1}\right)$$
$$e_N(2G_N + 4G_{N-1}) + 2e_{N-1}G_{N-1} = -6(C_N - C_{N-1}) + \\ + 6(C_a - C_N)\left(1 + \frac{G_{N-1}}{G_N}\right) \quad (2.6)$$

In the case $N = 3$ (three layers) we have equations (2.6) and (2.5) for $i = 2$.

Then

$$e_i = e_{i,1}C_1 + e_{i,2}C_2 + e_{i,3}C_3 + e_{i,0},$$

$$m_i = m_{i,1}C_1 + m_{i,2}C_2 + m_{i,3}C_3 + e_{i,0},\ i = 1;2;3 \quad (2.7)$$

From (2.2), (2.7) follows the system of three PDE

$$\begin{cases} D_{1x}\partial^2 C_1(x,y)/\partial x^2 + D_{1y}\partial^2 C_1(x,y)/\partial y^2 + \\ + 2H_1^{-1}e_1(x,y) + \widehat{F}_1(x,y) = 0 \\ D_{2x}\partial^2 C_2(x,y)/\partial x^2 + D_{2y}\partial^2 C_2(x,y)/\partial y^2 + \\ + 2H_2^{-1}e_2(x,y) + \widehat{F}_2(x,y) = 0 \\ D_{3x}\partial^2 C_3(x,y)/\partial x^2 + D_{3y}\partial^2 C_3(x,y)/\partial y^2 + \\ + 2H_3^{-1}e_3(x,y) + \widehat{F}_3(x,y) = 0 \end{cases} \quad (2.7)$$

where $\widehat{F}_i(x,y) = F_i(x,y) + 2H_1^{-1}e_{i,0},\ i = 1;2;3$. (2.3)

3 The Finite Difference method

For solving 2-D problems a uniform grid $\left(N_x \times (N_y+1)\right)$ is considered:

$$\omega_h = \left\{ \begin{array}{l} \left(x_i, y_j\right),\ x_i = ih_x,\ y_j = (j-1)h_y,\ i = \overline{1, N_x},\\ j = \overline{1, N_y + 1},\ N_x h_x = l,\ N_y h_y = L \end{array} \right\}$$

Subscripts (i, j) refer to x, y indices, the mesh spacing in the x_i, y_j directions are h_x and h_y. The PDEs (2.7) can be rewritten in following vector form:

$$D_x \partial^2 C / \partial x^2 + D_y \partial^2 C / \partial y^2 - AC + \widehat{F} = 0$$

(3.1)

where D_x, D_y are the 3-d order diagonal matrices with elements D_{1x}, D_{2x}, D_{3x} and D_{1y}, D_{2y}, D_{3y}, C is the 3 order vectors-column with elements C_1, C_2, C_3, $\widehat{F}$ is also the vectors-column with elements $\widehat{F}_1, \widehat{F}_2, \widehat{F}_3$, and matrix A is in following form:

$$A = -2 \begin{pmatrix} e_{1,1}/H_1 & e_{1,2}/H_1 & e_{1,3}/H_1 \\ e_{21}/H_2 & e_{22}/H_2 & e_{23}/H_3 \\ e_{3,1}/H_3 & e_{3,2}/H_3 & e_{3,3}/H_3 \end{pmatrix}.$$

The equation (3.1) with periodical conditions for vector function C in the uniform grid (x_i, y_j) is replaced by vector difference equations of second order approximation [4, 5].

They consist of vectors-columns and block-martices of order circulant symmetric matrixes.

The calculation of circulant matrix (matrix inversion and multiplication) can be carried out with MATLAB [2, 6]

The boundary conditions (1.5) are replaced by difference equations of first order approximation.

4 The numerical methods

The vectors-column W_j of vector difference equations is calculated by Thomas algorithm in the matrix form using MATLAB.

$$W_j = X_j W_{j+1} + Y_j = 0,\ j = N_y(-)1$$

(4.1)

where X_j, Y_j are corresponding matrices and vectors, obtaining of following expressions

$$X_j = \left(CC_j - AA_j X_{j-1}\right)^{-1} BB_j \quad ,$$

$$Y_j = \left(CC_j - AA_j X_{j-1}\right)^{-1} \left(AA_j Y_j + F_j\right), \quad j = 2(1)N_y$$

(4.2)

Here $X_1 = E \quad Y_1 = 0 \quad W_{\widehat{N}+1} = \left(E - X_{\widehat{N}}\right)^{-1} Y_{\widehat{N}}$, $\left(\widehat{N} = N_y\right)$ where

$$E = \begin{pmatrix} [1,0,...,0] & 0 & 0 \\ 0 & [1,0,...,0] & 0 \\ 0 & 0 & [1,0,...,0] \end{pmatrix}.$$

The inverse matrix of

$$A = \begin{bmatrix} A11 & A12 & A13 \\ A21 & A22 & A23 \\ A31 & A32 & A33 \end{bmatrix}$$

$B = A^{-1}, \left(BA = AB = E\right)$ is in the form

$$B = \begin{bmatrix} B11 & B12 & B13 \\ B21 & B22 & B23 \\ B31 & B32 & B33 \end{bmatrix}$$

where B is obtained due to MATLAB [6].

5. Approbation of numerical algorithms

We consider following test for the approbation of the calculations:

$f_1 = f_1 = f_1 = C_0 = 0$, $\alpha = 6D_{1z}$, $\alpha = 600D_{1z}$,

$C_a = C_{0a} \cos(\pi y / L) \sin(2\pi x / l)$, $C_{0a} = 1$.

The special solutions in the form $c_i(x, y, z) = g_i(z) \cos(\pi y / L) \sin(2\pi x / l),\ i = 1; 2; 3$ of the PDE (1.1) can be obtain from following boundary value problem for three ODE (for conditions (1.3, 1.4)):

$$g_1''(z) - a_1^2 g_1(z) = 0 \quad ,$$

$$D_{1z} g_1'(0) - \alpha\left(g_1(0) - C_0\right) = 0,$$

$$g_2''(z) - a_2^2 g_2(z) = 0,\ g_3''(z) - a_3^2 g_3(z) = 0,$$

$$g_3(Z) = C_{0a},\ g_1(H_1) = g_2(H_1),$$

$$D_{1z} g_1'(H_1) = D_{2z} g_2'(H_1),$$

$$g_2(L_1) = g_3(L_1),\ D_{2z} g_2'(L_1) = D_{3z} g_3'(L_1),$$

where $L_1 = H_1 + H_2$, $a_i = \pi \sqrt{\left(\frac{4D_{ix}}{l^2} + \frac{D_{iy}}{L^2}\right) / D_{iz}}$, $i = 1; 2; 3.$

Therefore the exact solution is

$$g_1(z) = P_1 \sinh(a_1 z) + P_0 \cosh(a_1 z),$$

$$g_2(z) = P_2 \sinh(a_2 z) + P_3 \cosh(a_2 z)$$

$$g_3(z) = P_4 \sinh(a_3 z) + P_5 \cosh(a_3 z),$$

where coefficients $P_i, i = \overline{0,5}$ are functions dependent of $a_i, i = \overline{1,3}$, D_{1z}, D_{2z}, D_{3z}, $\sinh(t), \cosh(t)$ (calculated for $t = a_1 H_1, a_2 H_1, a_2 L_1, a_3 L_1$), $\tanh(t), \coth(t)$ (calculated for $t = a_2 H_1, a_3 L_1$).

The averaged values are

$$C_1 = H_1^{-1}\int_0^{H_1} g_1(z)dz = \frac{1}{a_1 H_1}\cdot$$

$$\left(P_1\left(\cosh(a_1H_1)-1\right)+P_0\sinh(a_1H_1)\right)$$

$$C_2 = H_2^{-1}\int_{H_1}^{L_1} g_2(z)dz = \frac{1}{a_2 H_2}$$

$$\left(\begin{matrix}P_3\left(\sinh(a_2L_1)-\sinh(a_2H_1)\right)+\\ P_2\left(\cosh(a_2L_1)-\cosh(a_2H_1)\right)\end{matrix}\right)$$

$$C_3 = H_3^{-1}\int_{L_1}^{Z} g_3(z)dz = \frac{1}{a_3 H_3}$$

$$\left(\begin{matrix}P_5\left(\sinh(a_3Z)-\sinh(a_3L_1)\right)+\\ P_4\left(\cosh(a_3Z)-\cosh(a_3L_1)\right)\end{matrix}\right)$$

We have following numerical results $H_1=1, H_2=1.5, H_3=0.5, Z=3.0, C_0=0, C_{0a}=1$ for maximal and minimal values of c_k in the plane $z=z_k, z_k=(k-1)h_z, k=\overline{1,12}$, $z_{13}=Z$, $z_5=H_1$, $z_{11}=H_1+H_2$, $h_z=0.25$ by:

$D_{1z}=10^{-3}$, $D_{2z}=1.875\cdot10^{-3}$, $D_{3z}=0.1333\cdot10^{-3}$, $\alpha=600D_{1z}$ and $\alpha=6D_{1z}$, $D_{1x}=D_{1y}=3\cdot10^{-3}$, $D_{2x}=D_{2y}=4\cdot10^{-4}$, $D_{3x}=D_{3y}=5\cdot10^{-5}$

The numerical results by $N_x=N_y=20, N_z=12$ are given in the table 1 (c_{ap}, c_{an} are the approximate and analytical-exact values). We have following averaged (integral) values:

1) $\alpha=600D_{1z}$ - for C_{ap} : $C_1=0.0646$, $C_2=0.1894$, $C_3=0.6202$; for C_{an}: $C_1=0.0663$, $C_2=0.1931$, $C_3=0.6284$;

2) $\alpha=6D_{1z}$ - for C_{ap}: $C_1=0.1609$, $C_2=0.2545$, $C_3=0.6482$; for C_{an}: $C_1=0.1669$, $C_2=0.2617$, $C_3=0.6581$.

The numerical results for $N_x=N_y=40$ are coincided with 3 decimal places.

TABLE 1.

THE ANALYTICAL AND NUMERICAL RESULTS FOR 3 LAYERS (MAX. AND MIN. VALUES $\pm$)

z_k	$\alpha=600$	$\alpha=600$	$\alpha=6$	$\alpha=6$
	c_{ap}	c_{an}	c_{ap}	c_{an}
0.00	0.0020	0.0021	0.1206	0.1257
0.25	0.0328	0.0339	0.1395	0.1451
0.50	0.0642	0.0659	0.1599	0.1659
0.75	0.0963	0.0986	0.1820	0.1883
1.00	0.1292	0.1321	0.2057	0.2123
1.25	0.1476	0.1508	0.2196	0.2264
1.50	0.1671	0.1705	0.2350	0.2420
1.75	0.1877	0.1912	0.2521	0.2591
2.00	0.2096	0.2133	0.2709	0.2780
2.25	0.2331	0.2367	0.2917	0.2986
2.50	0.2578	0.2617	0.3142	0.3213
2.75	0.6189	0.6272	0.6469	0.6568

III RESULTS AND DISCUSSION

6. The numerical results

6.1. Determining of the difussion coefficients in the 1D case

In 1D case we have the boundary value problem of the following 3 ODEs

$c_1''(z)=0$, $c_2''(z)=0$, $c_3''(z)=0$,

$D_{1z}c_1'(0)-\alpha\left(c_1(0)-C_0\right)=0$, $c_3(Z)=C_{0a}$,

$c_1(H_1)=c_2(H_1)$, $D_{1z}c_1'(H_1)=D_{2z}c_2'(H_1)$,

$c_2(L_1)=c_3(L_1)$, $D_{2z}c_2'(L_1)=D_{3z}c_3'(L_1)$.

Using proportions $D_{1z}/D_{2z}=x_1$, $D_{1z}/D_{3z}=y_1$, $D_{1z}/\alpha=z_1$ $z1$ we have following solutions:

$c_1(z)=C_1z+C_2$,

$c_2(z)=C_3z+C_4$ $c_3(z)=C_5z+C_6$,

where $C_1=\dfrac{C_{0a}-C_0}{H_1+x_1H_2+y_1H_3+z_1}$,

$C_2=C_0+z_1C_1$, $C_3=x_1C_1$,

$C_4 = C_{0a} - C_1(L_1x_1 + y_1H_3)$, $C_5 = y_1C_1$,
$C_6 = C_{0a} - C_1y_1Z$.

From experimentally obtained data $c_1(0) = C_{00}$, $c_1(H_1) = C_{01}$, $c_2(L_1) = C_{02}$, we can determin the relations

$$x_1 = \frac{H_1(C_{02} - C_{01})}{H_2(C_{01} - C_{00})},\ y_1 = \frac{H_1(C_a - C_{02})}{H_3(C_{01} - C_{00})},$$
$$z_1 = \frac{H_1(C_{00} - C_0)}{(C_{01} - C_{00})}.$$

We consider the data for 2 metals in the peat blocks with $H_1 = 1, H_2 = 1.5, H_3 = 0.5$:

1) for Fe: $C_{0a} = 0.188$, $C_0 = 0, C_{00} = 0.66$, $C_{01} = 0.83$, $C_{02} = 1.50$ we get obtain

$D_{2z} = 0.38D_{1z}$, $D_{3z} = 0.22D_{1z}$, $\alpha = 0.26D_{1z}$,

2) for Ca: $C_{0a} = 4.63$, $C_0 = 0, C_{00} = 1.30$, $C_{01} = 1.90$, $C_{02} = 2.38$ we get obtain

$D_{2z} = 1.875D_{1z}$, $D_{3z} = 0.133D_{1z}$, $\alpha = 0.46D_{1z}$.

We obtain with MAPLE by $D_{1z} = 10^{-3}$ the figures (Fig. 1, 2) and the coefficients $C_1, C_2, C_3, C_4, C_5, C_6$ depending of C_{00}, C_{01}, C_{02}.

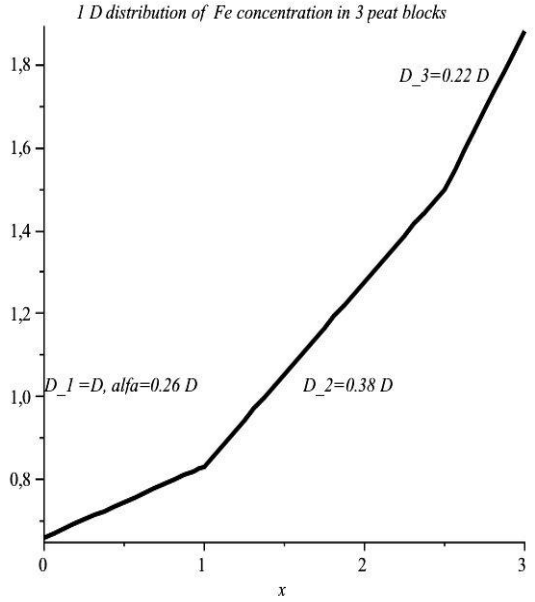

Fig. 1. Fe distribution and D_z

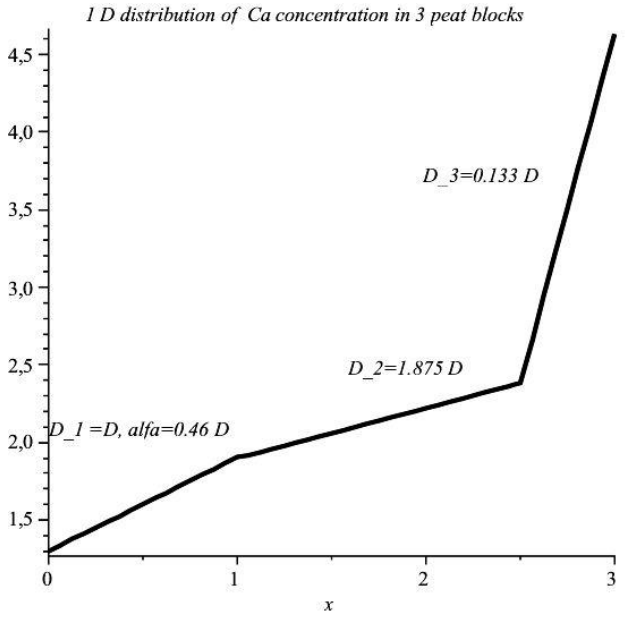

Fig. 2. Ca distribution and D_z

6.2. The calculation of concentration of metals in peat blocks

We consider the metals Fe and Ca concentration in the 3 layered peat blocks Ω with $L = l = 1m$ - dimensions of the block's base, $H_1 = 1m$, $H_2 = 1.5m$, $H_3 = 0.5m$, $L_1 = H_1 + H_2 = 2.5m$, $Z = H_1 + H_2 + H_3 = 3m$ - heights of the layers.

On the top of the earth $(z = Z)$ we have the measured concentration c mg/kg of metals in the following nine points in the (*x; y*) plane:

1) for Fe: *c*(01., 0.2) = 1.69*; c*(0.5, 0.2) = 1.83*; c*(0.9, 0.2) = 1.72*; c*(0.1, 0.5) = 1.70*; c*(0.5, 0.5) = 1.88*; c*(0.9, 0.5) = 1.71*; c*(0.1, 0.8) = 1.71*; c*(0.5, 0.8) = 1.82*; c*(0.9, 0.8) = 1.73,

2) for Ca:

c(0.1, 0.2) = 3.69*; c*(0.5, 0.2) = 4.43*; c*(0.9, 0.2) = 3.72*; c*(0.1, 0.5) = 4.00*; c*(0.5, 0.5) = 4.63*; c*(0.9, 0.5) = 4.11*; c*(0.1, 0.8) = 3.71*; c*(0.5, 0.8) = 4.50*; c*(0.9, 0.8) = 3.73.

This date are smoothing by 2D interpolation with MATLAB operator, using the spline function.

We have following diffusion coefficients in the layers:

1) for Fe: $(C_{00} = 0.66, C_{0a} = 1.88)$:

$D_{1z} = 10^{-3}$, $D_{2z} = 0.38 \cdot 10^{-3}$, $D_{3z} = 0.22 \cdot 10^{-3}$,

2) for Ca: $(C_{00} = 1.30, C_{0a} = 4.63)$:

$D_{1z} = 10^{-3}$, $D_{2z} = 1.875 \cdot 10^{-3}$, $D_{3z} = 0.1333 \cdot 10^{-3}$,

The diffusion coefficients in x, y directions are:

$D_{1x} = D_{1y} = 3 \cdot 10^{-4}$, $D_{2x} = D_{2y} = 4 \cdot 10^{-4}$,

$D_{3x} = D_{3y} = 5 \cdot 10^{-5}$ .///

In the Fig. 3, Fig. 4 graphics of metals concentration c depending of vertical coordinate z by $x = l/2,\ y = L/2$ and in other points are given.

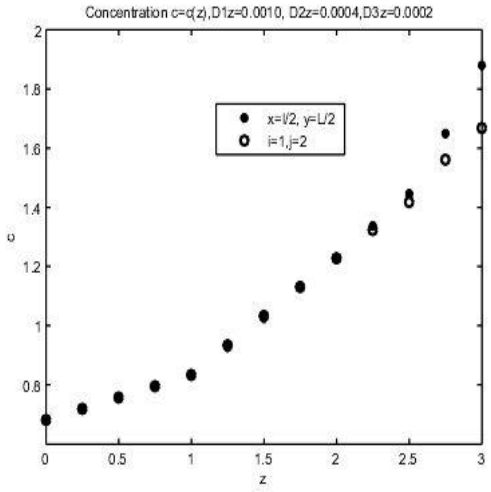

Fig. 3. Fe concentration *c* depending on z

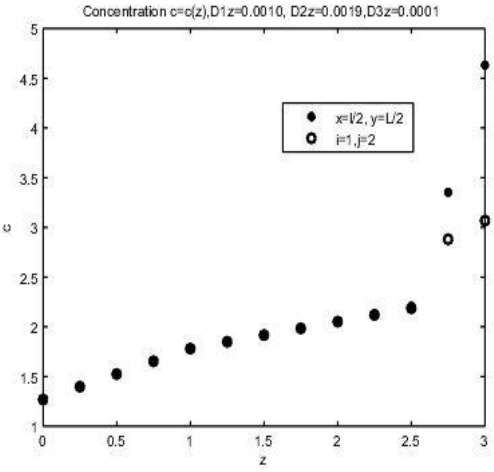

Fig. 4. Ca concentration *c* depending on z

The distribution of concentration c in the (x, y) plane is given: by $z = H_1$ (Fig. 5, 6.), $z = L_1 = H_1 + H_2$ (Fig. 7, 8.) $Z = H_1 + H_2 + H_3$ (Fig. 9, 10.).

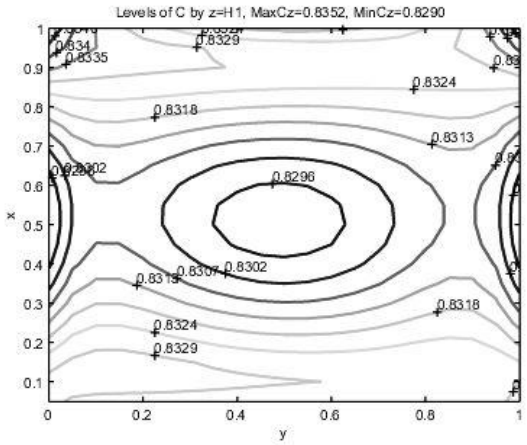

Fig. 5. Fe concentration *c* in the (x;y) plane by z=H1

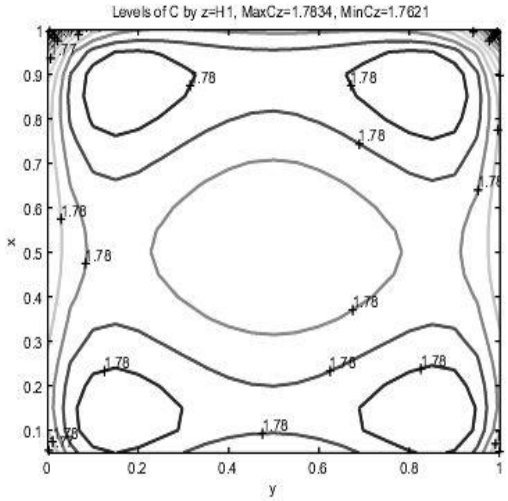

Fig.6. Ca concentration *c* in the (x;y) plane by z=H1

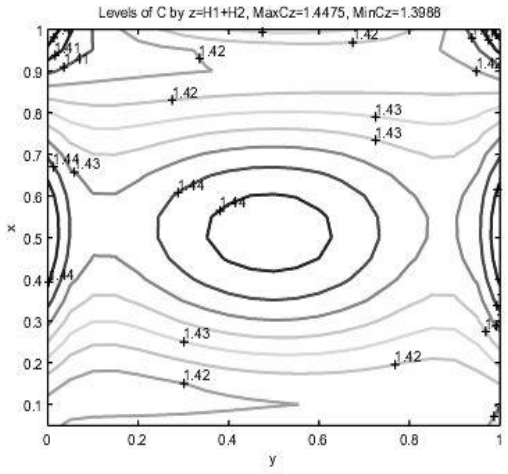

Fig. 7. Fe concentration *c* in the (x;y) plane by z=H1+H2

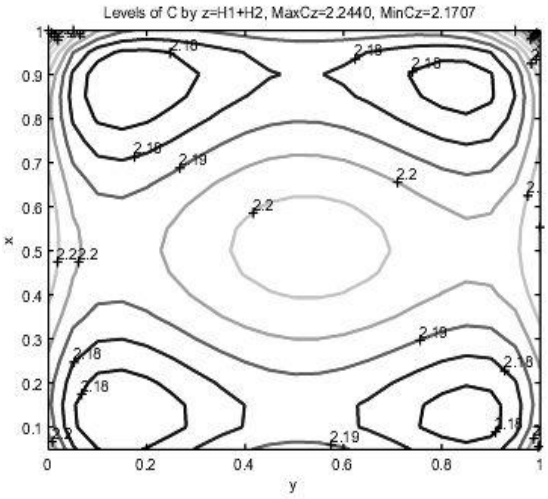

Fig. 8. Ca concentration *c* in the (x;y) plane by z=H1+H2

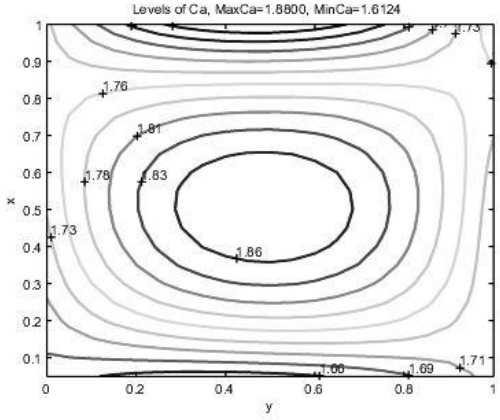

Fig. 9. Fe concentration *c* in the (x;y) plane by z=Z

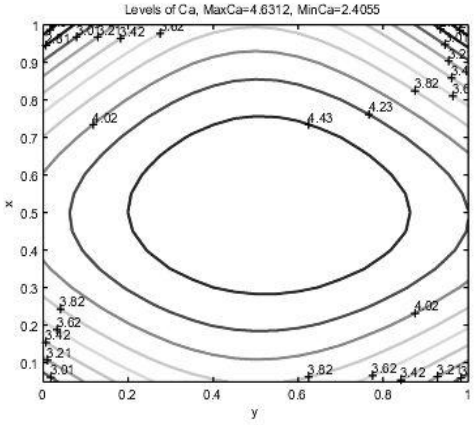

Fig. 10. Ca concentration *c* in the (x;y) plane by z=Z

The distribution of concentration c in the (z, x) plane by $y = L/2$ accordingly for Fe and Ca is given in Fig. 11, Fig. 12.

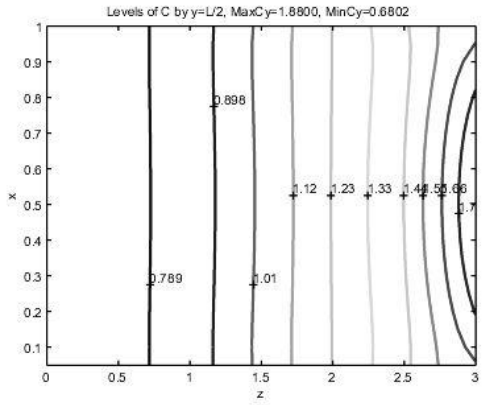

Fig. 11. Fe concentration *c* depending of vertical coordinate z by y=L/2

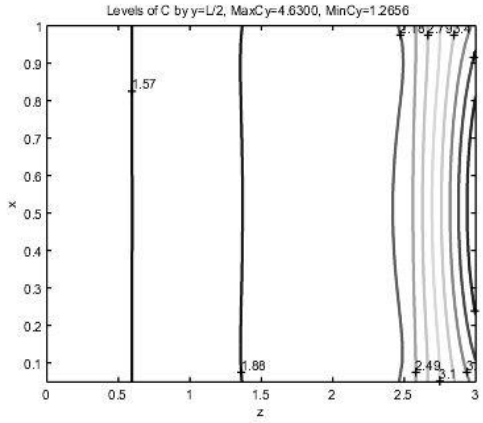

Fig. 12. Ca concentration *c* depending of vertical coordinate z by y=L/2

And the averaged values of concentration c in the second layer are given in Fig. 13, Fig. 14.

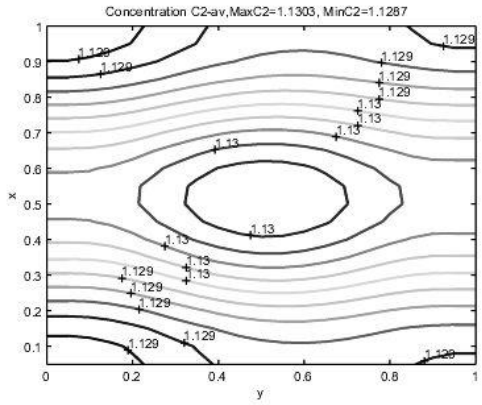

Fig. 13. Averaged values C2 in second layer for Fe concentration

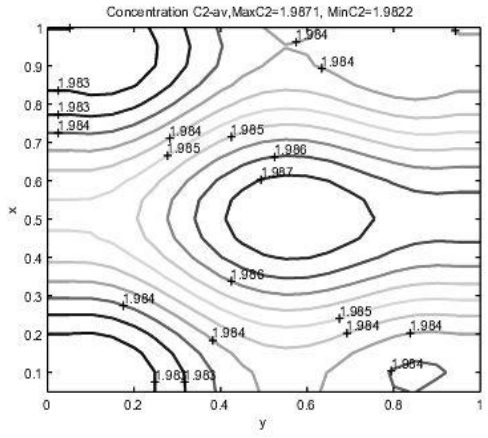

Fig. 14. Averaged values C2 in second layer for Ca concentration

IV Conclusion

The 3D diffusion problem in *N* layered domain described by a boundary value problem of the system of PDEs with piece-wise constant diffusion coefficients are approximate on the 2D boundary value problem of a system of *N* PDEs.

As opposed to the models analyzed previously [1,4], the newly established mathematical model envisages modeling mass transfer in N-layers, and the boundary conditions of the 3rd type included in the model enable the modeling of the substance flux through the boundary surface of the specified area in the direction of Earth's interior.

Test samples with an analytical solution (the indicator of transfer process) were developed and a numerical experiment was used to test and analyze the established method for three layers in comparison with the methods described previously.

The analytical and numerical results were coincided with 3 decimal places and it means that mathematical model have a practical application in real determination of trace elements concentrations.

The established mathematical model is applicable in studying transfer processes, where substance mass is transferred through boundary surfaces of the specified area, for instance, in a purification plant, purifying works etc.

V References

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