# ANALYTICAL SOLUTION FOR 3D MODEL OF PEAT BLOCKS

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**Abstract.** In this paper we consider averaging methods for solving the 3-D boundary value problem in domain containing peat blocks. We consider the metal concentration in the peat block. Using experimental data a mathematical model for calculation of the concentration of metal in different points in the peat layer is developed. A specific feature of these problems is that it is necessary to solve the 3-D boundary-value problems for elliptic type partial differential equations of the second order with piece-wise diffusion coefficients in every direction. The special exponential type spline, with interpolation middle integral values of piece-wise smooth function, is defined. This procedure allows reduces the 3-D problem to a problem of 2-D and 1-D problems and the solution of the approximated problem is obtained analytically. The solution of the corresponding averaged 2-D initial-boundary value problem is obtained numerically, using for approach differential equations, the discretization in space applying the central differences. The approximation of the 2-D non-stationary problem is based on the implicit finite-difference and alternating direction (ADI) methods. The numerical solution is compared with the analytical solution.

**Keywords:** diffusion problem, special splines, analytic and numerical solution.

## 1. Introduction

The task of sufficient accuracy numerical simulation of quick solution of 3-D problems for mathematical physics in multilayered media is important in known areas of the applied sciences. To achieve this goal we consider two methods: the special finite difference scheme and averaging method by using integral parabolic and exponential splines. For engineering calculation of the concentration of metal in a peat layered block the averaging method is chosen. The finite difference method is used only for solving the obtained 2-D problem. The layered peat blocks are modelled in [1; 2].

A.Buikis [3; 4] considers different assumptions for averaging methods along the vertical coordinate. These methods were applied for the mathematical simulation of the mass transfer process in multilayered underground systems.

It is necessary to solve the 3-D initial-boundary-value problems for parabolic type partial differential equations of the second order with piece-wise parameters in multilayer domain. The special spline, with interpolation middle integral values of piece-wise smooth function, is defined. With the help of these splines the problems of mathematical physics are reduced in 3-D with piece-wise coefficients to respect one coordinate analytically to problems for the system of equations in 2-D.

The solutions of the corresponding 2-D initial-boundary value problem are obtained numerically using the implicit finite difference approximation and the alterating method of Duglas and Rachford. The 3-D problem is reduced to 2-D and 1-D problems using integral parabolic and exponential splines.

## 2. Mathematical model of 3-D diffusion problem

The process of diffusion of the metal in the peat block is considered in 3-D parallelepiped:

$$\Omega = \left\{ (x, y, z) : 0 \le x \le L_x,\ 0 \le y \le L_y,\ 0 \le z \le L_z \right\}.$$

We will consider the nonstationary 3-D problem of the linear diffusion theory for homogenous materials. We will find the distribution of metal concentrations $c = c(x, y, z, t)$ in $\Omega$ at the point $(x, y, z) \in \Omega$ and at the time $t$ by solving the following 3-D initial-boundary value problem for partial differential equation (PDE):

$$\frac{\partial c(x, y, z, t)}{\partial t} = \frac{\partial}{\partial x}\left( D_x \frac{\partial c(x, y, z, t)}{\partial x} \right) + \frac{\partial}{\partial y}\left( D_y \frac{\partial c(x, y, z, t)}{\partial y} \right) + \frac{\partial}{\partial z}\left( D_z \frac{\partial c(x, y, z, t)}{\partial z} \right) + f(x, y, z, t),$$

$$x \in (0, L_x),\ y \in (0, L_y),\ z \in (0, L_z),\ t \in (0, t_f),\ \partial c(0, y, z, t)/\partial x = \partial c(x, 0, z, t)/\partial y = 0$$

$$D_z \partial c(x, y, 0, t)/\partial z - \beta_z \left( c(x, y, 0, t) - c_{0z}(x, y) \right) = 0,$$

$$D_x \partial c(L_x, y, z, t) / \partial x + \alpha_x \big(c(L_x, y, z, t) - c_{ax}(y, z)\big) = 0,$$

$$D_y \partial c(x, L_y, z, t) / \partial y + \alpha_y \big(c(x, L_y, z, t) - c_{ay}(x, z)\big) = 0,$$

$$D_z \partial c(x, y, L_z, t) / \partial z + \alpha_z \big(c(x, y, L_z, t) - c_{az}(x, y)\big) = 0,$$

$$c(x, y, z, 0) = c_0(x, y, z), \tag{2.1}$$

where $D_x$, $D_y$, $D_z$ – constant diffusion coefficients;
$\alpha_x$, $\alpha_y$, $\alpha_z$, $\beta_z$ – constant mass transfer coefficients given in the 3rd type boundary conditions;
$c_{0z}$, $c_{ax}$, $c_{ay}$, $c_{az}$ – given concentration values on the boundaries;
$t_f$ – the final time;
$c_0(x, y, z)$ – is the given initial concentration.

## 3. Averaged method in z-direction with the integral exponential type spline

Using the averaged method with respect to $z$ with exponential or hyperbolic trigonometric functions we have:

$$c_z(x, y, t) = L_z^{-1} \int_0^{L_z} c(x, y, z, t) dz,$$

$$c(x, y, z, t) = c_z(x, y, t) + m_z \frac{0.5 L_z \sinh(a(z - 0.5L_z))}{\sinh(0.5 a L_z)} + e_z \left( \frac{L_z^2}{4} \left( \frac{\sinh^2(a(z - 0.5L_z))}{\sinh^2(0.5 a L_z)} - A_z \right) \right),$$

where $A_z = \dfrac{\sinh(aL_z)/(aL_z) - 1}{\cosh(aL_z) - 1}$.

If a parameter $a > 0$ tends to zero, then we obtain the limit as a parabolic spline because of $A_z \to 1/3$ [3]:

$$c(x, y, z, t) = c_z(x, y, t) + m_z(x, y, t)(z - 0.5L_z) + e_z(x, y, t)\big((z - 0.5L_z)^2 - L_z^2/12\big).$$

It is possible to find out the unknown functions $m_z(x, y, t)$ and $e_z(x, y, t)$ from the boundary conditions (2.1) in the following form:

$$0.5 D_z L_z a_{0z}(m_z - e_z l_z) - \beta_z \big(c_z - 0.5 m_z L_z + e_z L_z A_{1z} - c_{0z}\big) = 0,$$

$$0.5 D_z L_z a_{0z}(m_z + e_z l_z) + \alpha_z \big(c_z + 0.5 m_z L_z + e_z L_z A_{1z} - c_{az}\big) = 0,$$

where $A_{1z} = 0.25 L_z (1 - A_z)$.

Then

$$m_z(x, y, t) = \big(\beta_z a_{22}(c_z(x, y, t) - c_{0z}(x, y, t)) + \alpha_z a_{12}(-c_z(x, y, t) + c_{az}(x, y, t))\big) / \det,$$

$$e_z(x, y, t) L_z = -c_z(x, y, t) g_z + c_{az}(x, y) a_z + c_{0z}(x, y) b_z,$$

$$g_z = (a_{11}\alpha_z + a_{21}\beta_z / \det), \; a_z = \alpha_z a_{11} / \det, \; b_z = \beta_z a_{21} / \det, \; \det = a_{11}a_{22} + a_{12}a_{21},$$

$$a_{11} = 0.5 L_z (D_z a_{0z} + \beta_z), \; a_{21} = 0.5 L_z (D_z a_{0z} + \alpha_z), \; a_{12} = 0.5 D_z a_{0z} L_z + \beta_z A_{1z},$$

$$a_{22} = 0.5 D_z a_{0z} L_z + \alpha_z A_{1z}, \; a_{0z} = a \coth(0.5 a L_z).$$

We obtain the initial-boundary value 2-D problem (3.1), where $B_z = D_z \alpha_{0z}$.

The initial-boundary value 2-D problem (2.1) is in the following form:

$$\begin{cases} \dfrac{\partial c_z(x,y,t)}{\partial t} = \dfrac{\partial}{\partial x}\left( D_x \dfrac{\partial c_z(x,y,t)}{\partial x}\right) + \dfrac{\partial}{\partial y}\left( D_y \dfrac{\partial c_z(x,y,t)}{\partial y}\right) - B_z g_z c_z(x,y,t) + f_z(x,y,t) + \\ + B_z\left(a_z c_{az}(x,y) + b_z c_{0z}(x,y)\right) \\ x \in (0, L_x),\ y \in (0, L_y),\ t \in (0, t_f), \partial c_z(0,y,t)/\partial x = \partial c_z(x,0,t)/\partial y = 0 \\ D_x \partial c_z(L_x, y, t)/\partial x + \alpha_x\left(c_z(L_x, y, t) - c_{ax}^v(y)\right) = 0 \\ D_y \partial c_z(x, L_y, t)/\partial x + \alpha_y\left(c_z(Lx, L_y, t) - c_{ay}^v(x)\right) = 0 \\ c_z(x,y,0) = c_{z,0}(x,y) \end{cases} \quad (3.1)$$

where $f_z(x,y,t) = L_z^{-1}\int_0^{L_z} f(x,y,z,t)dz$, $c_{ax}^v(y) = L_z^{-1}\int_0^{L_z} c_{ax}(y,z)dz$,

$c_{ay}^v(x) = L_z^{-1}\int_0^{L_z} c_{ay}(x,z)dz$, $c_{z,0}(x,y) = L_z^{-1}\int_0^{L_z} c_0(x,y,z)dz$.

## 4. Averaged method in *y*-direction

Using the averaged method with respect to $y$ with exponential or hyperbolic trigonometric functions we have

$$c_{z,y}(x,t) = L_y^{-1}\int_0^{L_y} c_z(x,y,t)dy$$

$$c_z(x,y,t) = c_{z,y}(x,t) + m_y \frac{0.5L_y \sinh(a(y-0.5L_y))}{\sinh(0.5aL_y)} + e_y\left(\frac{L_y^2}{4}\left(\frac{\sinh^2(a(y-0.5L_y))}{\sinh^2(0.5aL_y)} - A_y\right)\right),$$

with the unknown functions $m_y(x, t)$, $e_y(x, t)$, we can determine these functions from the boundary conditions (3.1) in the following form:

$$m_y(x,t) = e_y(x,t)L_y = -g_y\left(c_{z,y}(x,t) - c_{a,y}(x)\right),$$

where $a_{0y} = a\coth(0.5aL_y)$, $A_{1y} = 0.25L_y(1 - A_y)$, $A_y = \dfrac{\sinh(aL_y)/((aL_y)-1)}{\cosh(aL_y)-1}$,

$g_y = \alpha_y / \left(D_y L_y a_{0y} + \alpha_y(0.5L_y + A_{1y})\right)$.

Then the initial-boundary value problem (3.1) is in the following form

$$\begin{cases} \dfrac{\partial c_{z,y}(x,t)}{\partial t} = \dfrac{\partial}{\partial x}\left( D_x \dfrac{\partial c_{z,y}(x,t)}{\partial x}\right) - \left(g_z B_z + g_y B_y\right)c_{z,y}(x,t) + f_{z,y}(x,t) + \\ + B_z\left(a_z c_{az}^v(x) + b_z c_{0z}^v(x)\right) + B_y g_y c_{ay}^v(x), \quad x \in (0, L_x), t \in (0, t_f) \\ \partial c_{z,y}(0,t)/\partial x = 0, D_x \partial c_{z,y}(L_x, t)/\partial x + \alpha_x\left(c_{z,y}(L_x, t) - c_{ax}^{vv}(y)\right) = 0 \\ c_{z,y}(x,0) = c_{z,y,0}(x) \end{cases}, \quad (4.1)$$

where $B_y = D_y a_{0y}$, $f_{z,y}(x,t) = L_y^{-1}\int_0^{L_y} f_z(x,y,t)dy$, $c_{az}^v(x) = L_y^{-1}\int_0^{L_y} c_{az}(x,y)dy$,

$c_{0z}^v(x) = L_y^{-1}\int_0^{L_y} c_{0z}(x,y)dy$, $c_{ax}^{vv} = L_y^{-1}\int_0^{L_y} c_{ax}^v(y)dy$, $c_{z,y,0}(x) = L_y^{-1}\int_0^{L_y} c_{z,0}(x,y)dy$.

## 5. Averaged method in *x*-direction

It is possible to make averaging also with respect to $x$:

$$c_{z,y,x}(t) = L_x^{-1}\int_0^{L_x} c_{z,y}(x,t)dx$$

$$c_{z,y}(x,t) = c_{z,y,x}(t) + m_x \frac{0.5L_x \sinh(a(x-0.5L_x))}{\sinh(0.5aL_x)} + e_x\left(\frac{L_x^2}{4}\left(\frac{\sinh^2(a(x-0.5L_x)}{\sinh^2(0.5aL_x)} - A_x\right)\right)$$

with the unkown functions $m_x(t)$, $e_x(t)$, we can determine these functions from the boundary conditions (5.1) in the following form:

$$m_x(t) = e_x(t)L_x = (-g_x)\left(c_{z,y,x}(t) - c_{ax}^{vv}\right), A_x = \frac{\sinh(aL_x)/((aL_x)-1)}{\cosh(aL_x)-1},$$

where $g_x = \alpha_x / (D_x L_x a_{0x} + \alpha_x(0.5L_x + A_{1x})), a_{0x} = a\coth(0.5aL_x), A_{1x} = 0.25L_x(1-A_x)$.

Then the initial-boundary value problem (4.1) is in the following form

$$\begin{cases} \partial c_{z,y,x}(t)/\partial t = -(g_z B_z + g_y B_y + g_x B_x)c_{z,y,x}(t) + f_{z,y,x}(t) + B_z\left(a_z c_{az}^{vv} + b_z c_{0z}^{vv}\right) + \\ B_y g_y c_{ay}^{vv} + B_x g_x c_{ax}^{vv}, t \in (0, t_f), \quad c_{z,y,x}(0) = c_{z,y,x,0} \end{cases}, \quad (5.1)$$

where $f_{z,y,x}(t) = L_x^{-1}\int_0^{L_x} f_{z,y}(x,t)dx$, $c_{z,y,x,0} = L_x^{-1}\int_0^{L_x} c_{z,y,0}(x)dx$,

$c_{az}^{vv} = L_x^{-1}\int_0^{L_x} c_{az}^{v}(x)dx$, $c_{0z}^{vv} = L_x^{-1}\int_0^{L_x} c_{0z}^{v}(x)dx$, $B_x = D_x a_{0x}$.

Therefore, we have from (5.1) the initial problem for ODEs of the first order. The solution of this problem is

$$c_{z,y,x}(t) = \exp(-\gamma t)c_{z,y,x,0} + \int_0^t \exp(-\gamma(t-\xi))\overline{f}_{z,y,x}(\xi)d\xi, \quad (5.2)$$

where $\gamma = g_z B_z + g_y B_y + g_x B_x$,

$\overline{f}_{z,y,x}(t) = f_{z,y,x}(t) + B_z\left(a_z c_{az}^{vv} + b_z c_{0z}^{vv}\right) + B_y g_y c_{ay}^{vv} + B_x g_x c_{ax}^{vv}$.

For the averaged stationary solution follows the formula $c_{z,y,x} = \overline{f}_{z,y,x} / \gamma$ and we have the analytical solution for $c(x, y, z)$.

## 6. Analytical model for estimating the parameter a

We consider the special 1-D diffusion problem in the $z$-direction for:

$$f = \alpha_x = \alpha_y = 0, c_{az}(x,y) = C_a\cos(\pi x/L_x)\cos(\pi y/L_y),$$

$$c_{0z}(x,y) = C_0\cos(\pi x/L_x)\cos(\pi y/L_y).$$

Then the stationary solution of (2.1) is in the form

$$c(x,y,z) = c(z)\cos(\pi x/L_x)\cos(\pi y/L_y),$$

where the function $c(z)$ is the solution for the following boundary-value problem:

$$\begin{cases} \partial(\partial c(z)/\partial z)/\partial z - b^2 c(z) = 0, z \in (0, L_z), \quad D_z\partial c(0)/\partial z - \beta_z(c(0) - C_0) = 0, \\ D_z\partial c(L_z)/\partial z + \alpha_z(c(L_z) - C_a) = 0 \end{cases} \quad (6.1)$$

where $b = \pi\sqrt{(D_x/L_x^2 + D_y/L_y^2)/D_z}$.

Therefore, the exact solution is in the form $c(z) = P_1\sinh(bz) + P_2\cosh(bz)$, where the constants $P_1$, $P_2$ are the functions of $D_x$, $D_y$, $D_z$, $L_x$, $L_y$, $\alpha_z$, $\beta_z$, $C_0$, $C_a$. The averaged values are:

$$c^v = L_z^{-1}\int_0^{L_z} c(z)dz = (L_z b)^{-1}\left(P_1(\cosh(bL_z) - 1) + P_2\sinh(bL_z)\right).$$

The averaged method with respect to $z$ using exponential splines was compared with the sight worthy method. The following numerical results ($L_z = 3$, $C_0 = 0.3$, $C_a = 2.0$, $D_{1z} = 10^{-3}$, $D_x = D_y = 3\cdot10^{-4}$, $b = 2.4335$) for maximal error and averaged values depending on $a$, $\alpha_z$, $\beta_z$ were obtained. The numerical results are given in Table 1 ($a$ = 0 for parabolic spline) and the solution $c(z)$ for 3 methods ($\alpha_z = 20$, $\beta_z = 0$, $a = 2.3$) is represented in Fig. 1.

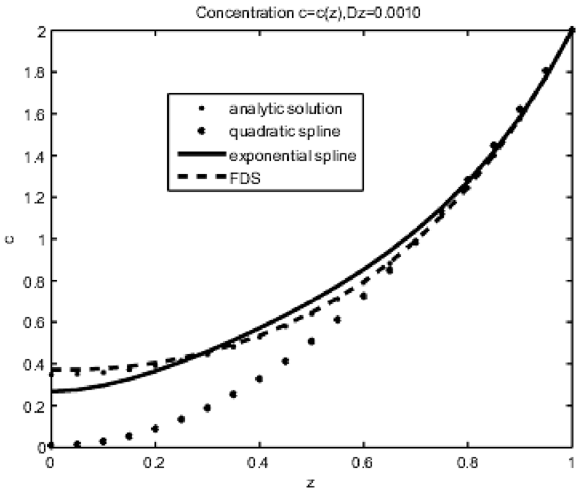


Fig. 1. **Solution $c(z)$ for $\alpha_z = 20, \beta_z = 0, a = 2.3$**

Table 1

**Maximal error $\delta$ and averaged values depending on $a$ for $\alpha_z$, $\beta_z$ $c_{an}^{v}$ – exact, $c_{ap}^{v}$ – approx**

| $\alpha_z$ | $\beta_z$ | a | δ | $c_{ap}^{v}$ | $c_{an}^{v}$ |
|---|---|---|---|---|---|
| 2 | 1 | 0.0 | 0.092 | 0.769 | 0.792 |
| - | - | 1.2 | 0.052 | 0.792 | - |
| - | - | 1.3 | 0.050 | 0.795 | - |
| - | - | 1.5 | 0.050 | 0.802 | - |
| 20 | 1 | 0.0 | 0.092 | 0.770 | 0.793 |
| - | - | 1.3 | 0.050 | 0.795 | - |
| 2 | 10 | 0.0 | 0.091 | 0.769 | 0.792 |
| - | - | 1.3 | 0.050 | 0.795 | - |
| 2 | 0 | 0.0 | 0.339 | 0.672 | 0.808 |
| - | - | 1.3 | 0.243 | 0.727 | - |
| - | - | 2.0 | 0.134 | 0.791 | - |
| - | - | 2.3 | 0.081 | 0.822 | - |

## 7. Some numerical results

A uniform grid in the space $((M + 1) \times (N + 1))$: $\{(y_i, x_j), y_i = (i - 1)hy, x_j = (j - 1)hx\}$, $i = \overline{1, M+1}$, $j = \overline{1, N+1}$, $M\ hy = L_y, N\ hx = L_x$ with a time $t$ moments $t_n = n\tau, n = 0,1,...$ was used for numerical approximation of the 2-D problem – therefore the grid function $U_{i,j}^{n} \approx c_z(x_j, y_i, t_n)$ was used for approximation of the concentration function $c_z(x, y, t)$.

For the grid function $U_{i,j}^{n}$ calculation Tomas algorithm in $x$ and $y$ directions was used for realization of the alternating direction method (ADI) of Douglas and Rachford (1955) and 3-point difference equations for every direction was constructed.

The numerical results are obtained for $z_m = mh_z$, $m = \overline{0, 10}$, $h_z = L_z / 10$, $D_x = D_y = 3\cdot10^{-4}$, $D_z = 10^{-3}$, $L_z = 3$, $L_x = L_y = 1$, $\alpha_z = 20$, $\beta_z = 10$, $\alpha_x = \alpha_y = 2.5$, $M = N = 20$, $a = 1.3$.

On the top of earth ($z = L_z$) the concentration c (mg·kg$^{-1}$) of metals is measured in the following nine points in the $(x, y)$ plane:

$$c(0.1, 0.2) = 3.69\,;\, c(0.5, 0.2) = 4.43\,;\, c(0.9, 0.2) = 3.72\,;$$

$$c(0.1, 0.5) = 4.00\,;\, c(0.5, 0.5) = 4.63\,;\; c(0.9, 0.5) = 4.11\,;$$

$$c(0.1, 0.8) = 3.71;\; c(0.5, 0.8) = 4.50;\; c(0.9, 0.8) = 3.73\,.$$

These data are smoothing in matrix $c_{az}$ by 2-D interpolation with MATLAB operator, using the spline function. In Fig. 2 we can see the distribution of the concentration $c$ for Ca in the $(x, y)$ plane by $z = L_z$. On the base of peat block $z = 0$ the elements of matrix $c_{0z}$ have a constant value 1.30 mg·kg$^{-1}$.

For the initial condition the averaged solutions $c_z(x, y)$ are chosen. We have the stationary solution with $\tau = 1$, $t_f = 1000$, $\tau = 1, t_f = 1000$ , the maximal error $10^{-6}$, the maximal value of $c_z(x, y)$ 2.6446 for averaged method 2.6892 for ADI method (following results can be seen in Fig. 2-5).

Depending on the number of the grid points ($N$, $M$) we have the following maximal values for the ADI method:

$$2.6974\ (M = N = 10),\ 2.6892\ (M = N = 20),\ 2.6859\ (M = N = 40),\ 2.6841\ (M = N = 60).$$

Depending on the parameter $a$ by ($M = N = 20$) it is possible to find out the following maximal values corresponding to the averaged and ADI methods:

$$2.6446;\ 2.6892\ (a = 1.3),\ 2.6172;\ 2.6406\ (a = 0.1),\ 2.6582;\ 2.7300\ (a = 2.0).$$

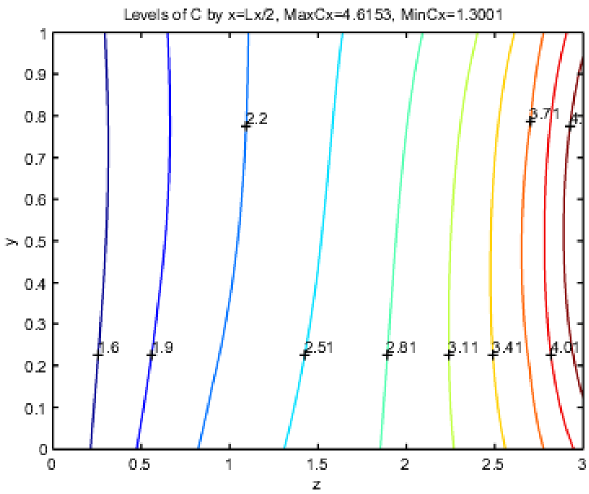


Fig. 2. **Levels of averaged concentration $c_z(x, y)$ for $x = L_x / 2$**

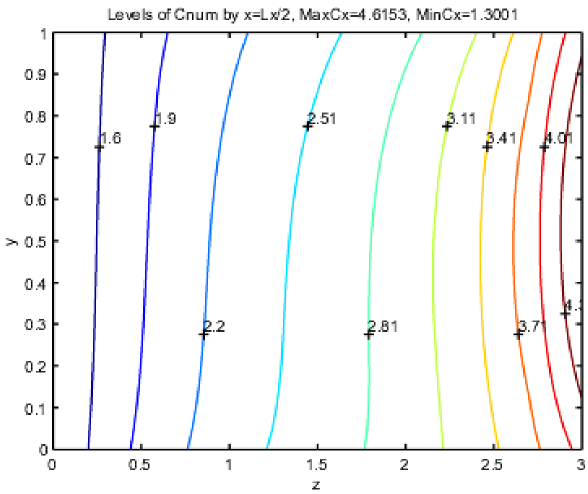


Fig. 3. **Levels of numerical concentration $c_z(x, y)$ for $x = L_x / 2$**

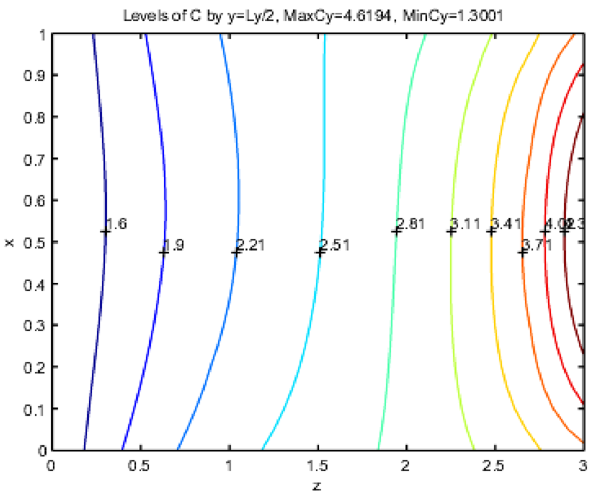


Fig. 4. **Levels of averaged concentration $c_z(x, y)$ for $y = L_y / 2$**

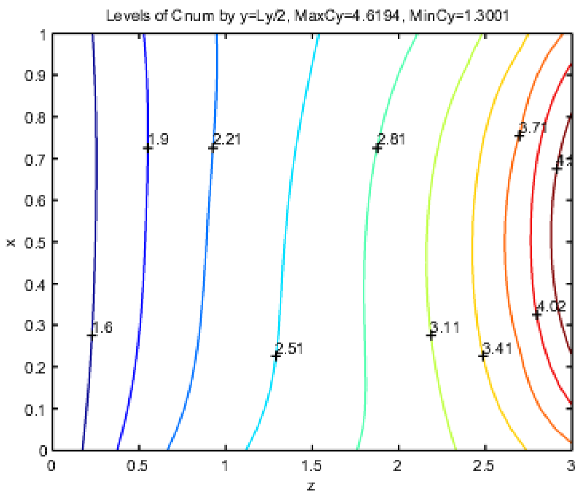


Fig. 5. **Levels of numerical concentration $c_z(x, y)$ for $y = L_y / 2$**

## 8. Conclusions

The 3-D diffusion problem in peat blocks is reduced to 2-D and 1-D problems using the integral parabolic and exponential splines. The 1-D problem is solved analytically. For the exponential spline the best parameter for minimal error is calculated.

The solutions of the corresponding averaged non stationary 2-D initial-boundary value problem are obtained numerically using the alternating-direction implicit (ADI) method of Douglas and Rachford. The numerical solution is compared with the analytical solution.

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