NUMERICAL ANALYSIS FOR SYSTEM OF PARABOLIC EQUATIONS WITH PERIODIC FUNCTIONS

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Abstract. Solving of parabolic partial differential equations (PDE) is closely connected to many practical studies of mathematical physics, environmental science, chemistry, etc. – modelling of heavy metal distribution in peat layer's block; solving heat transfer problems in multilayer environments. Despite the current great capabilities of software, the development of accurate and effective numerical technique algorithms is still ongoing, particularly in areas 2-D and 3-D involving periodic boundary conditions (PBC). The solutions of some linear and nonlinear problems for parabolic type equations and systems with (PBCs) are obtained using the method of lines (MOL) to approach the partial differential equations (PDS) in the time and discretization in space applying the finite difference scheme (FDS) and the finite difference scheme with the exact spectrum (FDSES). As an application of the described mathematical models the 3-D diffusion problem of peat block is solved. The FDS method in the uniform grid is used to approximate the differential operator of the second and the first order derivatives in the space, using multi-point stencil. The solution in the time is obtained analytically with continuous and discrete Fourier methods and numerically, using MATLAB.

Keywords: analytical solutions, circulant matrices, finite difference schemes, Fourier series, heat transfer equations, linear and nonlinear systems.

1. Introduction

A periodic function $y = f(x)$, having a period L, can be represented as $f(x + L) = f(x)$.

In the 2-D problem which depends on time t, the second argument t is not discretized and the method of lines (MOL) is used to solve such problems with given initial conditions at $t = 0$.

In the source [1] the finite-difference scheme (FDS) for local approximation of periodic function's derivatives in a $2n + 1$ point stencil is studied, obtaining higher order accuracy approximation. This method in the uniform grid with N mesh points is used to approximate the differential operator of the second order and the first order derivatives in the space, using the multi-point stencil.

It is shown that the eigenvalues of FDS matrix representation A can be obtained as a sum whose terms do not depend on n. This allows easily solving FDS by the spectral decomposition of A.

In recent decades, parabolic partial equations have been intensively developed, as many researchers have used them in chemistry, biology, etc. Periodic semi-linear parabolic partial equations are interesting because they can explain the seasonal variation of the phenomena seen in the models [2-4].

The described methods are applicable for solving of various problems of mathematical physics involving periodical functions and periodic boundary conditions (PBCs), for example, the 3-D diffusion problem of peat block [5], the 2-D problem for the system of magnetohydrodynamic (MHD) equations along with the heat transfer equation for the viscous electrically conducting incompressible liquid-electrolyte by moving between infinite cylinders placed periodically [6; 7], the method for representing periodic functions and enforcing exactly PBCs for solving differential equations with deep neural networks [8], the novel discrete differential operators for periodic functions of one and two-variables [8; 9].

The solutions of some problems of partial differential equations (PDE) with PBCs are obtained, using the method of lines (MOL) to approach PDEs in the time and for discretization them in the space, applying FDS of a different order of the approximation and the finite difference scheme with FDSES.

Here the FDS method in the uniform grid is used to approximate the differential operator of the second order and the first order derivatives in the space, using the multi-point stencil. The solution in the time is obtained analytically with continuous and discrete Fourier methods and numerically, using MATLAB solver "ode 15s", "pdepe".

2. Materials and methods

In the chapter 2.1 a multi-point stencil for local approximation of periodic function derivatives, as the theoretical basis for performing numerical experiments, is studied.

PDEs and heat transfer equations with convection are widely represented in mathematically oriented scientific fields such as physics and engineering. For example, they underlie today's scientific understanding of heat, diffusion, convection, thermodynamics and fluid dynamics.

It should be noted that it is in many cases more difficult to analyse heat transfer by convection (create a Math Model, run numerical experiments, interpret the results obtained) compared to heat transfer in a particular material (environment) [6; 11].

Being based on the theoretical and practical possibilities of mathematics applications we study the following PDEs- heat transfer equations with convection (chapters 2.2-2.8):

1. linear heat transfer equation (1) is given in chapter 2.2, solution with the Fourier method (chapter 2.3) and the corresponding discrete method FDS and FDSES (chapter 2.4) [10; 11] for solving them are studied;
2. linear system of heat transfer equations (5) is given in chapter 2.5 and the corresponding solution with the Fourier method (chapter 2.6) with its matrix form (chapter 2.7) is considered;
3. nonlinear system of heat transfer equations (8) is given in chapter 2.8, its discrete solution in matrix form is obtained numerically. Since the exact solution of the equation (8) cannot be found, the changes in the maximum and minimum values of the found numerical solutions are compared depending on the parameters used.

Possible uses of equations (1), (5) and (8): combustion processes (plaster plates, wheat straw pellets); reaction-diffusion equations for the combustion process, such as a nonstationary and nonlinear physical model for chemical reaction with temperature and with reaction-diffusion equations; nonlinear heat transfer equations [11].

There is an increasing number of researches into the environmental impact of various sources of natural origin – atmospheric deposits, soil dust and aerosols, surface drainage water, as well as anthropogenic sources – atmospheric particles, wastewater, industrial emissions, etc.

Although some heavy metals (e.g. Fe, Ca), which are part of trace elements, play an important role in the world of plants and animals, their high concentrations become dangerous for any form of life.

Chapter 4 therefore studies the distribution of concentrations of metal Ca in the peat block by solving the 3-D initial boundary value problem for PDEs (10) with PBC in two directions.

2.1. Multi-point stencil for approximate differential operator of the second and the first order derivatives

We start with describing methods for higher order accuracy approximation of a smooth from the space $C_{2n+2}[0, L]$ function in an interval $[0; L]$. Consider the uniform grid $x_j = jh$, $j = \overline{0, N}$, $Nh = L$. Let n be natural number, satisfying $2n + 1 \leq N$.

PBCs allows to freely increase approximation order by increasing the stencil of grid points. In the case of $2n + 1$ point stencil we have to use additional conditions of periodicity $u_r = u_{N+r}$, $r \in [-n, n]$. This way algorithms with higher order precision FDS can be obtained.

Similarly [1], we use multi-point stencil to approximate derivatives of the second and the first order respect to space argument x, (u', u'') in the uniform grid.

We consider the finite difference approximation for the second order derivative $-u''(x_j)$ using the uniform grid $x_j = jh$ with $2n + 1$ points stencil $(x_{j-n},\ldots x_{j-1}, x_j, x_{j+1},\ldots, x_{j+n})$.

Then we have $O(h^{2n})$ order of approximation in the following form:

$$u''(x_j) = \frac{1}{h^2}\sum_{k=-n}^{n} C_k u(x_{j-k}) + E_n \frac{h^{2b} u^{(2n+2)}(\xi)}{(2n+2)!}, x_{j-n} < \xi < x_{j+n}.$$

Using properties of symmetry

$$C_m = C_{-m}, C_0 = -2\sum_{m=1}^{n} C_m$$

and to determine the other coefficients C_m, ($m > 0$), we get the system of linear algebraic equations with the Van-der-monde matrix:

$$C_m = \frac{2(n!)^2(-1)^{m-1}}{m^2(n-m)!(n+m)!}$$

If $m = 2n + 2$ then

$$E_n = -2\sum_{m=1}^{n} C_m m^{2n+2}.$$

In this case the finite difference matrix A for the second order derivative approximation $-u''(x_j)$ is circulant N order matrix in the form [11].

$$A = -\frac{1}{h^2}[C_0, C_1, ..., C_n, 0, ..., 0, C_n, C_{n-1}, ..., C_2, C_1].$$

The eigenvalues of the matrix A are [1]

$$\mu_k = \frac{4}{h^2}\sum_{m=1}^{n} Q_m \sin^{2m}\frac{\pi k}{N}$$

where the coefficients

$$Q_m = \frac{2((m-1!))^2(4)^{m-1}}{(2m)!}$$

are not depending on n.

Using the first derivative $u'(x_j)$ for the higher order approximation $O(h^{2n})$ we have the following circulant matrix representation:

$$A^0 = -\frac{1}{h}[0, c_1, c_2, ..., c_n, 0, ..., 0, -c_n, -c_{n-1}, ..., -c_2, -c_1]$$

where

$$c_m = \frac{(n!)^2(-1)^{m-1}}{m(n-m)!(n+m)!}, m = \overline{1, n}.$$

Then the eigenvalues are imaginary ($i = \sqrt{-1}$);

$$\mu_k^0 = \frac{2i}{h}\sum_{m=1}^{n} c_m \sin\frac{2\pi mk}{N} = \frac{2i}{h}\sin\frac{2\pi k}{N}\sum_{m=1}^{n} q_m \sin^{2m-2}\frac{\pi k}{N},$$

where

$$q_m = \frac{2((m!))^2 4^{m-1}}{m(2m)!}$$

are not depending on n.

2.2. Heat transfer eq8uation with convection

$$\frac{\partial T(x,t)}{\partial t} = K_0\frac{\partial^2 T(x,t)}{\partial x^2} + P_0\frac{\partial T(x,t)}{\partial x} + f(x,t). \quad (1)$$

With the periodic boundary conditions

$$T(0,t) = T(L,t), \frac{\partial T(0,t)}{\partial x} = \frac{\partial T(L,t)}{\partial x}, t \in (0, t_b),$$

where K_0 – const > 0, P_0 = const > 0 are real coefficients;
$T(x,0) = T_0(x)$, $f(x,t)$, $T_0(x)$ – initial condition – periodic functions with the period L,
t_b – final time.

2.3. Solution with Fourier method

We can use the Fourier method for solving the initial-boundary value problem in the form

$$T(x,t)=\sum_{k\in Z}a_k(t)w^k(x),\ f(x,t)=\sum_{k\in Z}b_k(t)w^k(x)$$

where

$$w^k(x)=\sqrt{\frac{1}{L}}\exp\left(\frac{2\pi ikx}{L}\right), w^k(x)=\sqrt{\frac{1}{L}}\exp\left(-\frac{2\pi ikx}{L}\right)=w^{-k}(x);$$

$\left(w^k,w^m\right)=\int_0^L w^k(x)w^m(x)dx=\delta_{k,m}$ – orthonormed eigenvectors $b_k(t) = (f,w^k(x))$.

Then for the unknown functions $a_k(t)$ get the complex initial value problem for ODEs of the first order:

$$\begin{cases}\dot{a}_k(t)+a_k(t)\lambda_k=b_k(t)\\ a_k(0)=\dfrac{1}{L}\displaystyle\int_0^L T_0(s)\exp\frac{-2i\pi ks}{L}ds\\ b_k(t)=\dfrac{1}{L}\displaystyle\int_0^L f(s,t)\exp\frac{-2i\pi ks}{L}ds\end{cases}\tag{2}$$

where

$$\lambda_k=K\left(\frac{2\pi k}{L}\right)^2-\frac{2i\pi kP}{L}$$

The solution of (2) is

$$a_k(t)=\exp(-\lambda_k t)a_k(0)+\int_0^T\exp(\lambda_k(t-s))b_k(s)ds$$

The solution with the Fourier method can be obtained in real form

$$f(x,t)=\sum_{k=1}^{\infty}\left(b_{kc}(t)\cos\frac{2\pi kx}{L}+b_{ks}(t)\sin\frac{2\pi kx}{L}\right)+\frac{b_{0c}(t)}{2},$$

where

$$b_{kc}(t)\frac{2}{L}\int_0^L f(s,t)\cos\frac{2\pi ks}{L}ds, b_{ks}(t)\frac{2}{L}\int_0^L f(s,t)\sin\frac{2\pi ks}{L}ds.$$

Therefore, the solution is in real form:

$$T(x,t)=\sum_{k=1}^{\infty}\left(a_{kc}(t)\cos\frac{2\pi kx}{L}+a_{ks}(t)\sin\frac{2\pi kx}{L}\right)+\frac{a_{0c}(t)}{2},$$

where the coefficients $a_{kc}(t)$, $a_{ks}(t)$ can be obtained from the following initial boundary value problem of the system of two ODEs:

$$\begin{cases}\dot{a}_{kc}(t)+a_{kc}(t)\mathrm{Re}(\lambda_k)+a_{ks}(t)\mathrm{Im}(\lambda_k)=b_{kc}(t)\\ \dot{a}_{ks}(t)+a_{ks}(t)\mathrm{Re}(\lambda_k)-a_{kc}(t)\mathrm{Im}(\lambda_k)=b_{ks}(t)\end{cases}$$

$$a_{kc}(0)=\frac{2}{L}\int_0^L T_0(s)\cos\frac{2\pi ks}{L}ds$$

$$a_{ks}(0)=\frac{2}{L}\int_0^L T_0(s)\sin\frac{2\pi ks}{L}ds$$

$$\mathrm{Re}(\lambda_k)=K\frac{4\pi^2k^2}{L^2}, \mathrm{Im}(\lambda_k)=-P\frac{2\pi k}{L}$$

2.4. Discrete method

For the discrete problem we have the system of N ODEs in the form

$$\dot{U}(t) + K_0 AU(t) - P_0 A^0 U(t) = F(t), U(0) = U_0 \tag{4}$$

where A, A^0 – 3-diagonal circulant matrices of N order, with the eigenvalues μ_k, μ_k^0;
$U(t)$, $\dot{U}(t)$, U_0, $F(t)$ – column-vectors of N order.

We can also use the matrix representation $A = WDW^*$, $A^0 = WD^0W^*$,

where D, D^0 – diagonal-matrices with the elements μ_k, μ_k^0, $k = \overline{1, N}$.

For FDSES we can replace the eigenvalues in the diagonal-matrices in a special way ($N_2 = N/2$) [12]:

$$d_k = \frac{4\pi^2 k^2}{L^2} \text{ for } k = \overline{1, N_2} \text{ and } d_k = \frac{4\pi^2 (N-k)^2}{L^2} \text{ for } k = \overline{N_2, N}$$

$$d_k^0 = \frac{2\pi i k}{L} \text{ for } k = \overline{1, N_2} \text{ and } d_k^0 = -\frac{2\pi i (N-k)}{L} \text{ for } k = \overline{N_2, N}$$

For the column-vector $F(t)$ elements $f_j(t)$ we obtain

$$f_j(t) = \sum_{k=1}^{*N_2} \left(b_{kc}(t)\cos\frac{2\pi kj}{N} + b_{ks}(t)\sin\frac{2\pi kj}{N} \right) + \frac{b_{0c}(t)}{2},$$

where

$$b_{kc}(t)\frac{2}{N}\sum_{j=1}^{N} f_j(t)\cos\frac{2\pi kj}{N}, b_{ks}(t)\frac{2}{N}\sum_{j=1}^{N} f_j(t)\sin\frac{2\pi kj}{N}, k = \overline{1, N_2},$$

$$b_{0c}(t) = b_{Nc}(t) = \frac{2}{\sqrt{N}}, b_{N_{2,c}}(t) = \frac{2}{N}\sum_{j=1}^{N} \cos(\pi j),$$

$$N_2 = \frac{N}{2}, b_{N_2 s}(t) = b_{Ns}(t) = 0, \sum_{k=1}^{*N_2} \beta_k = \sum_{k=1}^{N_2 - 1} \beta_k + \frac{\beta_{N/2}}{2}$$

For the solution

$$u_j(t) = \sum_{k=1}^{*N_2} \left(a_{kc}(t)\cos\frac{2\pi kj}{N} + a_{ks}(t)\sin\frac{2\pi kj}{N} \right) + \frac{a_{0c}(t)}{2}$$

and

$$u_j(0) = \sum_{k=1}^{*N_2} \left(a_{kc}(0)\cos\frac{2\pi kj}{N} + a_{ks}(0)\sin\frac{2\pi kj}{N} \right) + \frac{a_{0c}(t)}{2}$$

with

$$u_j(t) = \sum_{k=1}^{*N_2} \left(a_{kc}(t)\cos\frac{2\pi kj}{N} + a_{ks}(t)\sin\frac{2\pi kj}{N} \right) + \frac{a_{0c}(t)}{2}$$

$$a_{kc}(0) = \frac{2}{N}\sum_{j=1}^{N_2} u_j(0)\cos\frac{2\pi kj}{N}, a_{ks}(0) = \frac{2}{N}\sum_{j=1}^{N_2} u_j(0)\sin\frac{2\pi kj}{N}$$

we need to determine the unknown functions $a_{kc}(t)$, $a_{ks}(t)$ f the following expressions:

$$f_j(t) = \dot{u}_j + K_0 (Au)_j - P_0 \left(A^0 u\right)_j =$$

$$= \sum_{k=1}^{*N_2} \left(\dot{a}_{kc}(t)\cos\frac{2\pi kj}{N} + \dot{a}_{ks}(t)\sin\frac{2\pi kj}{N} \right) + \frac{\dot{a}_{Nc}(t)}{2} +$$

$$+ K_0 \sum_{k=1}^{*N_2} \left(a_{kc}(t)\mu_k \cos\frac{2\pi kj}{N} + a_{ks}(t)\mu_k \sin\frac{2\pi kj}{N} \right) -$$

$$-P_0\sum_{k=1}^{*N_2}\left(-a_{kc}(t)\mu_k^0\cos\frac{2\pi kj}{N}+a_{ks}(t)\mu_k\sin\frac{2\pi kj}{N}\right)$$

From orthonormed conditions follows:

$$\frac{2}{N}\sum_{j=1}^{N}\cos\frac{2\pi kj}{N}\sin\frac{2\pi mj}{N}=\delta_{k,m},\ \frac{2}{N}\sum_{j=1}^{N}\sin\frac{2\pi kj}{N}\sin\frac{2\pi mj}{N}=\delta_{k,m},$$
$$\frac{2}{N}\sum_{j=1}^{N}\cos\frac{2\pi kj}{N}\cos\frac{2\pi mj}{N}=\delta_{k,m}$$

and to determine the functions $a_{kc}(t)$, $a_{ks}(t)$ we obtain the systems of ODEs (3), where the eigenvalues λ_k are replaced with the discreate eigenvalues

$$K_0\mu_k-P_0\mu_k^0,k=\overline{1,N}\,.$$

2.5. Linear system of heat transfer equations

We consider the linear system of M-heat transfer equation in the following form:

$$\frac{\partial T(x,t)}{\partial t}=K\frac{\partial^2 T(x,t)}{\partial x^2}+P\frac{\partial T(x,t)}{\partial x}+f(x,t) \tag{5}$$

with the periodic boundary conditions

K – positive definite M-order matrix with the elements $k_{m,s},m,s=\overline{1,M}$ and with different positive eigenvalues $\mu_k > 0$;

P is the real M-order matrix with the elements $p_{m,s},m,s=\overline{1,M}$ and with different real eigenvalues μ_P;

$T(x,0) = T_0(x)$,$f(x,t)$,$T(x,t)$,$T_0(x)$ – periodic functions column-vectors of the M-order.

2.6. Solution with Fourier method

We can use the Fourier method for solving the initial-boundary value problem in the real form:

$$T(x,t)=\sum_{k=1}^{\infty}\left(a_{kc}(t)\cos\frac{2\pi kx}{L}+a_{ks}(t)\sin\frac{2\pi kx}{L}\right)+\frac{a_{0c}(t)}{2}$$

where $a_{kc}(t)$, $a_{ks}(t)$ – unknown column-vectors of M-order.

We obtain the initial boundary value problem for the system of 2M- ODEs:

$$\begin{aligned}
\dot a_{kc}(t)&=-\lambda_k Ka_{kc}(t)+\lambda_k^0 Pa_{ks}+b_{kc}(t),\\
\dot a_{ks}(t)&=-\lambda_k Ka_{ks}(t)-\lambda_k^0 Pa_{kc}+b_{ks}(t),\\
a_{kc}(0)&=\frac{2}{L}\int_0^L T_0(s)\cos\frac{2\pi ks}{L}ds\\
a_{ks}(0)&=\frac{2}{L}\int_0^L T_0(s)\sin\frac{2\pi ks}{L}ds
\end{aligned} \tag{6}$$

where

$$b_{kc}(t)=\frac{2}{L}\int_0^L f(s,t)\cos\frac{2\pi ks}{L}ds,a_{ks}(t)=\frac{2}{L}\int_0^L f(s,t)\sin\frac{2\pi ks}{L}ds$$
$$\lambda_k=\frac{4\pi^2k^2}{L^2},\lambda_k^0=\frac{2\pi k}{L}.$$

For FDS with

$$T(x_j,t)\approx u_j(t),\ f_j(t)=f(x_j,t),\ j=\overline{1,N}$$

we obtain the system of vector-difference equations:

$$\dot{u}_j(t) = -K\Lambda u_j(t) + P\Lambda^0 u_j(t) + f_j(t), u_j(0) = T_0(x_j),$$

where u_j – M-order column-vector with the elements $u_j^m, m = \overline{1,M}$;

Λ, Λ_0 – the difference operators defined in the 2n-points stencil ($x_{j-n},\ldots,x_j,\ldots,x_{j+n}$), with the order of approximation (h^{2n}):

$$\Lambda u_j^m(t) = \frac{1}{h^2}\left(C_n\left(u_{j-n}^m(t) + u_{j+n}^m(t)\right) + \ldots + C_1\left(u_{j-1}^m(t) + u_{j+1}^m(t)\right) + C_0 u_j^m(t)\right),$$

$$\Lambda^0 u_j^m(t) = \frac{1}{h}\left(c_n\left(u_{j+n}^m(t) - u_{j-n}^m(t)\right) + \ldots + c_1\left(u_{j+1}^m(t) - u_{j-1}^m(t)\right)\right),$$

$$C_0 = -2\sum_{k=1}^{n} C_k, m = \overline{1,M}.$$

We have 2 circulant matrices:

$$-\Lambda = A = -\frac{1}{h^2}\left[C_0, C_1, \ldots, C_n, 0, \ldots, 0, C_n, C_{n-1}, \ldots, C_2, C_1\right],$$

$$\Lambda^0 = A^0 = \frac{1}{h}\left[0, c_1, c_2, \ldots, c_n, 0, \ldots, 0, -c_n, -c_{n-1}, \ldots, -c_2, -c_1\right],$$

which can be also represented in the form $A = WDW^*$, $A^0 = WD^0W^*$,

where D, D^0 – diagonal-matrices with the elements μ_k, μ_k^0, $k = \overline{1,N}$.

In this form we can consider FDSES. In the real form we have

$$u_j(t) = \sum_{k=1}^{*N_2}\left(a_{kc}(t)\cos\frac{2\pi kj}{N} + a_{ks}(t)\sin\frac{2\pi kj}{N}\right) + \frac{a_{0c}(t)}{2}$$

where $a_{kc}(t)$, $a_{ks}(t)$ – M-order column-vectors.

2.7. Solution in matrix form

We can write difference equations in the matrix form

$$\dot{u}(t) = \left(-K \otimes A + P \otimes A^0\right)u(t) + f(t), \tag{7}$$

where MN-order matrices

$$K \otimes A = \begin{pmatrix} k_{1,1}A & \ldots & k_{1,M}A \\ \ldots & \ldots & \ldots \\ k_{M,1}A & \ldots & k_{M,M}A \end{pmatrix}, P \otimes A^0 = \begin{pmatrix} p_{1,1}A^0 & \ldots & p_{1,M}A^0 \\ \ldots & \ldots & \ldots \\ p_{M,1}A^0 & \ldots & p_{M,M}A^0 \end{pmatrix}$$

are defined with Kroneker-tensor product;
$u(t)$, $u(0)$, $f(t)$ – MN column-vectors with the elements

$$u_j^m(t), u_j^m(0), f_j^m, m = \overline{1,M}, j = \overline{1,N}.$$

Matrices can be represented in the form $A = WDW^*$, $A^0 = WD^0W^*$, and solved by Matlab (operator “kron”).

For real representation we can use

$$A\cos_k = \mu_k \cos_k, A^0 \cos_k = -\left|\mu_k^0\right|\sin_k,$$

$$A\sin_k = \mu_k \sin_k, A^0 \sin_k = \left|\mu_k^0\right|\cos_k,$$

where $\sin_k$, $\cos_k$ – N-order vectors with the elements

$$\sin\frac{2\pi kj}{N}, \cos\frac{2\pi kj}{N}.$$

We have orthonormed conditions

$$\sum_{j=1}^{N} \sin_k \cos_k = \sum_{j=1}^{N} \sin_k \sin_k = \sum_{j=1}^{N} \cos_k \cos_k = \frac{N}{2}\delta_{k,s}\,.$$

Then for fixed frequency k of oscillations the solution can be found in the form

$$u(t) = d_s(t)\sin_k + d_c(t)\cos_k$$

where $d_s(t)$, $d_c(t)$ – unknown vector-functions of the time.

Then

$$\begin{aligned}
&\dot{u}(t) = \dot{d}_s(t)\sin_k + \dot{d}_c(t)\cos_k\,,\\
&Au(t) = \mu_k\left(d_s(t)\sin_k + d_c(t)\cos_k\right),\\
&A^0u(t) = \left|\mu_k^0\right|\left(d_s(t)\cos_k - d_c(t)\sin_k\right).
\end{aligned}$$

2.8. Nonlinear system of heat transfer equations

We consider the nonlinear system of M-heat transfer equation in the following form:

$$\frac{\partial T(x,t)}{\partial t} = K\frac{\partial^2 g_1(T(x,t))}{\partial x^2} + P\frac{\partial g_2(T(x,t))}{\partial x} + g_3(T(x,t)) \tag{8}$$

with the periodic boundary conditions, $g_1(T) = T^{\alpha}$, $g_2(T) = T^{\beta}$, $g_1(T) = T^{\gamma}$ are the power functions.

The discrete equations are in the form

$$\dot{u}(t) = (-K \otimes A)u^{\alpha}(t) + \left(P \otimes A^0\right)u^{\beta}(t) \tag{9}$$

3. Results and discussion

In the present chapter we have solved the heat transfer equation (1) and the discreate form (4), the linear system of two heat transfer equations (5) and the nonlinear system of two heat transfer equations (8) for fixed parameters. Also, as an example according to the above mentioned theoretical guidelines, we have solved the 3-D diffusion problem of peat block.

3.1. Results for linear system of ODE (4)

For (1) and (4) we consider the following parameters:

$$\begin{aligned}
&K_0 = 2, P_0 = -5, L = 1, T_0(x) = B_1\sin(2\pi x) + B_2\cos(2\pi x)\\
&f(t,x) = A_1(t)\sin(2\pi x) + A_2(t)\cos(2\pi x)\\
&B_1 = 0, B_2 = -1, A_1 = 5_2 = -10.
\end{aligned}$$

The solution is in the form

$$u(t,x) = d_1(t)\sin(2\pi x) + d_2(t)\cos(2\pi x)$$

and we obtain 2 ODEs:

$$\begin{cases}\dot{d}_1(t) = -4K_0\pi^2 d_1(t) - P_0 2\pi d_2(t) + A_1(t), d_1(0) = B_1\\ \dot{d}_2(t) = -4K_0\pi^2 d_2(t) - P_0 2\pi d_1(t) + A_2(t), d_2(0) = B_2\end{cases}$$

or in the system

$$\dot{d}(t) = Ad(t) + Gd(t), \text{ for vectors } d(0), G(t)$$

with the coordinates B_1, B_2; $A_1(t)$, $A_2(t)$ and matrix

$$A_0 = \begin{pmatrix} -4K_0\pi^2 & -2P_0\pi \\ 2P_0\pi & -4K_0\pi^2 \end{pmatrix}.$$

This system can be solved by MATLAB solver "ode15s".

We obtain the discrete solution from (4), where U_0, $F(t)$ are the N-order column-vectors with the elements $B_1\sin(2\pi x_j) + B_2\cos(2\pi x_j)$ and $A_1(t)\sin(2\pi x_j) + A_2(t)\cos(2\pi x_j)$.

We obtain the following maximal errors for N = 10 depending on the approximation order of derivatives $u''(x)$, $u'(x)$: 0.0050($O(h^2)$), 0.0039($O(h^4)$), $2.3\cdot10^{-5}$($O(h^6)$), $1.8\cdot10^{-6}$($O(h^8)$), $2.5\cdot10^{-8}$(*FDSES*).

It is seen that the maximal error in using the FDS method ($1.8\cdot10^{-6}$) is two order higher than the FDSES method ($2.5\cdot10^{-8}$). In Fig. 1 we can see the solution $u(t,x)$ by $N = 10$, with the periodical conditions by $x = 0$, $x = 1$ and maximal value $u(0.5,0) = 1$, $u(0.5,t) = -d_2(t) > 0$.

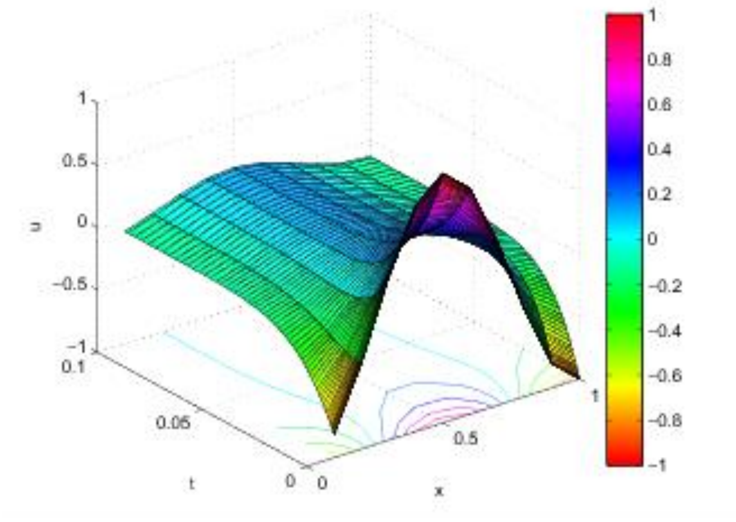

Fig. 1. **Solution *u*(*t*,*x*) by *N* = 10**

3.2. Results for linear system of two heat transfer equations (5)

We have an example: $M = 2$, $L = 1$, $t_b = 0.1$, $T_0{}^1(x) = B_{1,1}\sin(2\pi x) + B_{1,2}\cos(2\pi x_j)$, $T_0{}^2(x) = B_{2,1}\sin(2\pi x) + B_{2,2}\cos(2\pi x_j)$, $f^1(x,t) = A_{1,1}(t)\ \sin(2\pi x) + A_{1,2}(t)\ \cos(2\pi x)$, $f^2(x,t) = A_{2,1}(t)\ \sin(2\pi x) + A_{2,2}(t)\ \cos(2\pi x)$, $B_{1,1} = 0$, $B_{1,2} = 1$, $B_{2,1} = -1$, $B_{2,2} = 0$, $A_{1,1} = 5$, $A_{1,2} = 10$, $A_{2,1} = -10$, $A_{2,2} = -5$, and we can consider 2 matrices

$$\tilde{B} = \begin{pmatrix} B_{1,1} & B_{1,2} \\ B_{2,1} & B_{2,2} \end{pmatrix}, \tilde{A} = \begin{pmatrix} A_{1,1} & A_{1,2} \\ A_{2,1} & A_{2,2} \end{pmatrix}.$$

Matrices

$$K = \begin{pmatrix} 2 & -3 \\ -1 & 4 \end{pmatrix}, P = \begin{pmatrix} 2 & -5 \\ 1 & -4 \end{pmatrix}$$

with the eigenvalues $\lambda_K = (1;5)$, $\lambda_P = (1;-3)$.

We find the solution in the form

$$T^1(x,t) = d_{1,2}(t)\sin(2\pi x) + d_{1,2}(t)\cos(2\pi x),\ T^2(x,t) = d_{2,1}(t)\sin(2\pi x) + d_{2,2}(t)\cos(2\pi x),$$

then we obtain 4 ODEs for solving the coefficients $d_{1,1}$, $d_{2,1}$, $d_{2,1}$, $d_{2,2}$:

$$\dot{d}(t) = A_2 d(t) + F(t), d(0) = d_0,$$

where the matrix

$$A_2 = \begin{pmatrix} -4\pi^2 K & -2\pi P \\ 2\pi P & -4\pi^2 K \end{pmatrix},$$

4-order column-vectors are

$$d = (d_{1,1}, d_{2,1}, d_{2,1}, d_{2,2})^T,\ d(0) = (B_{1,1}, B_{2,1}, B_{2,1}, B_{2,2})^T,\ F = (A_{1,1}, A_{2,1}, A_{2,1}, A_{2,2})^T.$$

We have the following maximal errors for solutions T^1, T^2 (Table 1):

Table 1

Maximal errors for solutions T^1, T^2

Max. errors	**FDS**								**FDSES**	
	$O(h^2)$		$O(h^4)$		$O(h^6)$		$O(h^8)$			
	$N = 10$	$N = 20$	$N = 10$	$N = 20$	$N = 10$	$N = 20$	$N = 10$	$N = 20$	$N = 10$	$N = 20$
T^1	0.0071	0.0017	0.0113	0.0028	$8.3 \cdot 10^{-6}$	0.0016	$5.6 \cdot 10^{-8}$	$2.1 \cdot 10^{-7}$	$5.3 \cdot 10^{-8}$	$9.9 \cdot 10^{-8}$
T^2	0.0032	0.0008	0.0043	0.0011	$8.5 \cdot 10^{-6}$	0.0006	$6.1 \cdot 10^{-7}$	$2.6 \cdot 10^{-7}$	$2.0 \cdot 10^{-8}$	$9.6 \cdot 10^{-8}$

The maximal error using the FDS method, with increasing the number of grid points (from $N = 10$ to $N = 20$) under orders $O(h^6)$ and $O(h^8)$, increases, while using the FDSES method, increasing of N does not change the error's round.

In Fig. 2-4 we can see the matrix coefficients $d(t)$ depending on t and the solutions depending on x and t (in Fig. 2 the coefficients tend to stationary solution already by $t = 0.1$; in Fig. 3, Fig. 4 we can see different behaviour of the solutions u_1 and u_2).

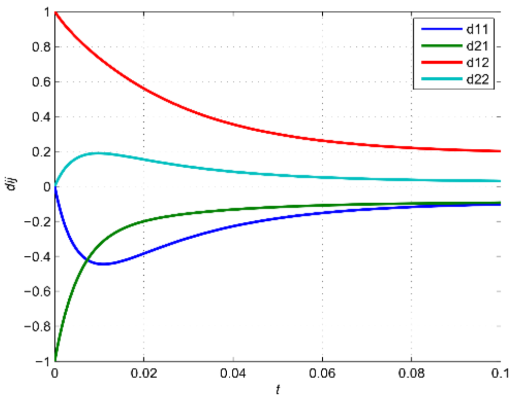

Fig. 2. **Matrix coefficients $d(t)$ depending on t, $N = 20$**

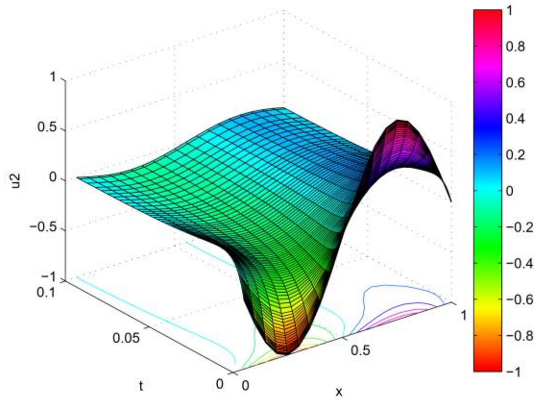

Fig. 3. **Solution $T^1(x,t)$**

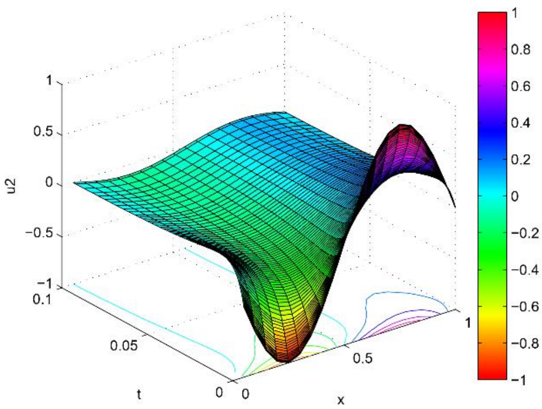

Fig. 4. **Solution $T^2(x,t)$**

3.3. Results for nonlinear system of two heat transfer equations (8)

For equation (8) we have following maximal (Mv_1, Mv_2) and minimal (mv_1, mv_2) values of solutions $v_1 = u_1$, $v_2 = u_2$ for $M = 2$, $t_b = 10$ depending on t (Table 2):

1. $\alpha = \beta = 3$, $\gamma = 2$ (in Fig. 5 we have symmetric, periodic oscillations in the space, the solution is stationary).

Table 2

Max-min values of $\pm u_1$, $\pm u_2$

Max-min values	N = 40					N = 80	
	FDS				FDSES	FDS	FDSES
	$O(h^2)$	$O(h^4)$	$O(h^6)$	$O(h^8)$		$O(h^8)$	
$\pm u_1$	0.17752	0.17755	0.17686	0.17715	0.17715	0.17723	0.17723
$\pm u_2$	0.10843	0.10847	0.10791	0.10822	0.10822	0.10827	0.10827

We can see that with increasing of an accuracy of the solution, it tends to constant values – $u_{1\,=\,\pm}$ 0.17723, $u_2 = \pm\, 0.10827$, using both studied methods.

2. In Fig. 6 we can see results by $\alpha = \beta = 3$, $\gamma = 2$, $L = 3$, $N = 80$ (solution slowly tends to stationary, only by $t = 20$).
3. In the next Fig. 7, Fig. 8 there are represented results by $\alpha_1 = 5$, $\alpha_2 = 3$, $\beta = 3$, $\gamma = 2$, $L = 3$, $N = 40$, $t_b = 5$ for 0.1·K with eigenvalues (0.1; 0.5), where $g_1(T) = [T^{(\alpha 1)}, x \in [1,N], T^{(\alpha 2)}, x \in [N + 1,2N]]$.

We can see the oscillations in time (in Fig. 7 there are solutions v_1, v_2 by $t = 5$). We obtain the following maximal values u_1, u_2 depending on $n = 1,2,3,4$ and for FDSES: 1.5461; 0.9288, $O(h^2)$, 1.4914; 0.8911, $O(h^4)$, 1.5061; 0.8969, $O(h^6)$, 1.4919;0.8894 $O(h^8)$, 1.5081; 0.8945 (FDES).

It can be seen that, with increasing the precision (order $O(h^8)$), the solution with the FDS method tends at a solution obtained by the FDSES method with error approximately 1.2% (u_1), 0.6% (u_2).

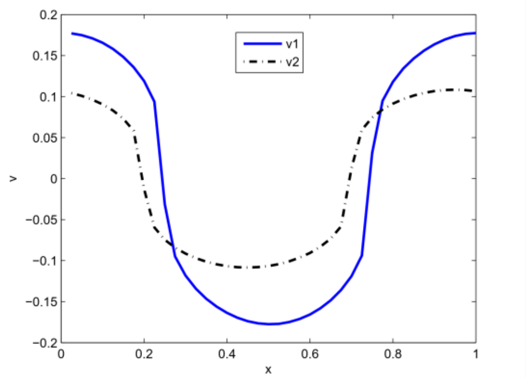

Fig. 5. **Solutions by t_b = 10, N = 40 depending on x**

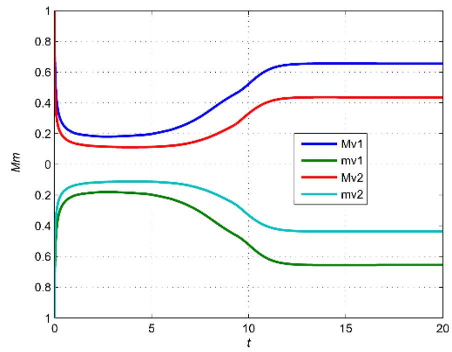

Fig. 6. **Maximal and minimal values depending on t, L = 3**

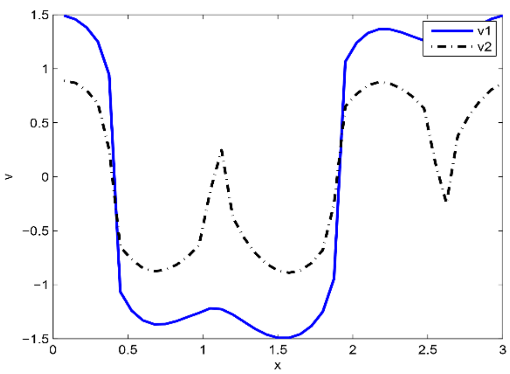

Fig. 7. **Solutions by t_b = 5, L = 3 depending on x**

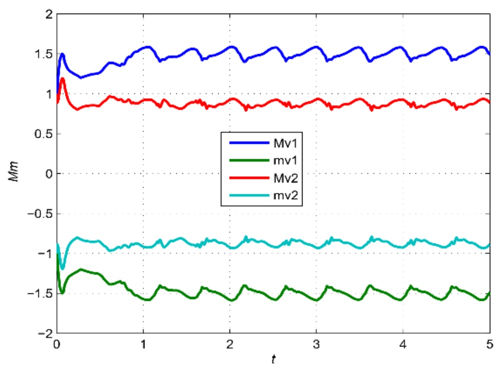

Fig. 8. **Maximal and minimal values depending on t**

4. Solution of 3-D diffusion problem of peat block

In [5] the concentration of metals Fe and Ca in the layered peat blocks is investigated. Using the experimental data, the mathematical model for calculation of concentration of metals in peat layers are developed. It is necessary to solve the 3-D boundary-value problems for PDEs with periodical boundary condition in one (x) direction.

We develop here a method for solving of a problem of one peat block with periodical boundary condition in two (x, y) directions.

The process of diffusion is considered in 3-D parallelepiped

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

We will find the distribution of concentrations of metals Ca in the peat block $c = c(x,y,z,t)$

by solving the following 3-D initial boundary value problem for partial differential equation (PDEs):

$$\begin{aligned}
&\frac{\partial c}{\partial t} = \frac{\partial}{\partial x}\left(D_x \frac{\partial c}{\partial x}\right) + \frac{\partial}{\partial y}\left(D_y \frac{\partial c}{\partial y}\right) + \frac{\partial}{\partial z}\left(D_z \frac{\partial c}{\partial z}\right),\\
&t \in (0, t_f), x \in (0, L_x), y \in (0, L_y), z \in (0, L_z),\\
&c(0, y, z, t) = c(L_x, y, z, t), \frac{\partial c(0, y, z, t)}{\partial x} = \frac{\partial c(L_x, y, z, t)}{\partial x},\\
&c(x, 0, z, t) = c(x, L_y, z, t), \frac{\partial c(x, 0, z, t)}{\partial y} = \frac{\partial c(x, L_y, z, t)}{\partial y},\\
&c(x, y, L_z, t) - c_{az}(x, y) = 0, D_z \frac{\partial c(x, 0, z, t)}{\partial y} - \alpha(c(x, y, 0, t) - c_{0z}(x, y)) = 0,\\
&c(x, y, z, 0) = c_0(x, y), t \in (0, t_b),
\end{aligned} \tag{10}$$

where D_x, D_y, D_z – the constant diffusion coefficients;
α – constant mass transfer coefficient at z = 0;
$c_{az}(x,y)$, $c_{0z}(x,y)$, $c_0(x,y)$ – given concentration on the boundary $z = 0$, $z = L_z$ and at the time $t = 0$;
t_b – final time, in x and y direction we have periodical BCs.

We consider the solution in the following form:

$$c(x,y,z,t) = C(z,t)f_1(x)f_2(y), c_{az} = C_{az}f_1(x)f_2(y), c_{0z} = C_{0z}f_1(x)f_2(y), c_0 = C_0f_1(x)f_2(y), L_x = L_y = 1,$$

where $f_1(x) = a_1(\sin(2\pi x) + \cos(2\pi x))$, $f_1(x) = a_2(\sin(2\pi y) + \cos(2\pi y))$,

Then we have following 1-D initial boundary value problem in z-direction:

$$\begin{cases}
\dfrac{1}{D_z}\dfrac{\partial C(z,t)}{\partial t} = -a_0^2 C(z,t) + \dfrac{\partial^2 c(z,t)}{\partial z^2}, z \in (0, L_z)\\
C(L_z, t) - C_{az} = 0, D_z \dfrac{\partial C(0,t)}{\partial z} - \alpha(C(0,t) - C_{0z}), t \in (0, t_b), c(z,0) = C_0,
\end{cases} \tag{11}$$

where $a_0^2 = \dfrac{4\pi^2(D_x + D_y)}{D_z}$.

Using a uniform grid with the number of the grid points $N_x = N_y = 10$, $N_z = 20$ we can define the finite difference matrix A of N_z-order and solved the discreate ODEs system (11) by MATLAB routine "pdepe".

The numerical results are obtained for [5]:

$t_b = 6$ s, $C_{az} = 4.63$ mg·m^{-3}, $C_{0z} = 1.13$ mg·m^{-3}, $\alpha = 200$ m·s^{-1}, $D_z = 10^{-3}$ m^2·s^{-1}, $L_x = L_y = 1$ m, $L_z = 3$ m, $D_z = D_y = 3\cdot10^{-4}$ m^2·s^{-1}, $a_1 = a_2 = 0.1$, $C_0 = ((C_{az} - C_{0z}) \cdot z/L_z) + C_{0z}$.

The stationary solution C(z) for (11) we can obtain also analytically by solving the following boundary-value problem for ODEs of second order:

$$\begin{cases} -a_0^2 C(z) + \dfrac{d^2 C(z)}{dz^2} = 0, z \in (0, L_z) \\ C(L_z) = C_{az}, D_z \dfrac{dC(0)}{d_z} - \alpha(C(0) - C_{0z}) = 0 \end{cases}$$

The solution is $C(z) = A_1 \sinh(a_0 z) + A_2 \cosh(a_0 z)$, where

$$A_1 = \frac{C_{az} - C_{0z}\cosh(a_0 L_z)}{\sinh(a_0 L_z) + \dfrac{a_0 D_z \cosh(a_0 L_z)}{\alpha}}, A_2 = C_{0z} + \frac{A_1 a_0 D_z}{\alpha}.$$

There are represented the stationary solution $C(z)$ (Fig. 9), and the solution depending on t, z (Fig. 10).

Changes of concentrations have similar characters – concentrations of Ca very fast decrease with the depth increasing from 4.63 to 1.13 $mg \cdot m^{-3}$. Major concentrations of heavy metals are observed at the top layers of peat.

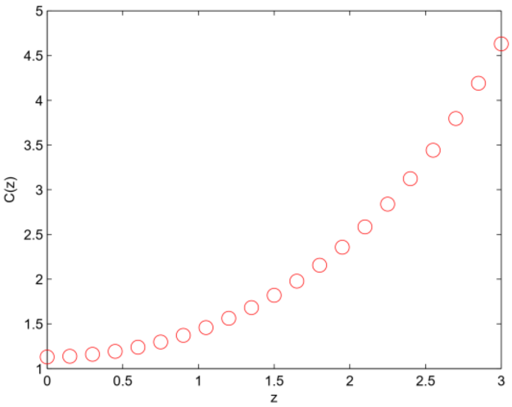

Fig. 9. **Stationary solution C(z)**

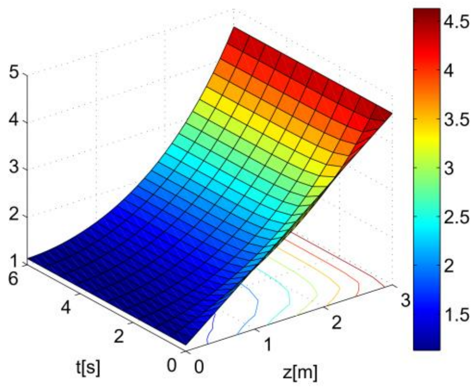

Fig. 10. **Nonstationary solution *C*(*t*,*z*)**

Conclusions

1. For higher order of approximation in space the differential operators multi-points stencil is used: for the second and first order derivatives with approximation $O(h^{2n})$, with N grid points and with $2n + 1 \leq N$ points stencil, circulant N-order matrices and eigenvalues are obtained.
2. The considered methods illustrate the simplicity and flexibility of finite-difference schemes: FDS with higher order approximation and FDSES with exact spectrum. For linear equations, regardless of the number of grid points, the FDSES method yielded a more accurate solution than the FDS method - the order of maximal error for equation (1) using the FDS method is two times higher than the FDSES method.
3. For linear system equations (5) the maximal error using the FDS method, with increasing the number of grid points N, increases, while using the FDSES method, increasing of N does not change the error's order (see Table 1).
4. For nonlinear system equations (8) with increasing of an accuracy of the solution, the maximal and minimal values of solutions tend to constant values using both studied methods (see Table 2). It can be seen that, with increasing the precision of FDS, the solution with the FDS method tends to a solution obtained by the FDSES method with error approximately 1.0%.
5. The effectivity of above-mentioned methods – FDS and FDSES for PBC is obtained by using circulant matrices, which simplified computational algorithms, and thus allowed a significant reduction in the amount of calculations to be performed.
6. MATLAB routines "ode15s" and "pdepe" were used for solving linear and nonlinear systems of parabolic type equations, which allowed to obtain the solutions of 1-D stationary and nonstationary boundary value problems.

7. 3-D diffusion problem of metal concentration in the peat block with PBC (10) is reduced to 1-D initial boundary values problem (11) using two fixed functions in x, y directions. Numerical experiment, using MATLAB routine “pdepe”, showed that the nonstationary solution (depending on (z,t)) of the above mentioned 1-D problem tends to its stationary solution (depending on z). It provides new information for further studies on the performance of measurements of heavy metal concentrations in peat.

Author contributions

The contribution of all three authors to the development of a given publication is equivalent.

All authors have read and agreed to the published version of the manuscript.

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