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Special Splines of Exponential Type for the Solutions of Mass Transfer Problems in Multilayer Domains

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Abstract. We consider averaging methods for solving the 3-D boundary-value problem of second order in multilayer domain.
The special hyperbolic and exponential type splines, with middle integral values of piece-wise smooth function interpolation are considered. With the help of these splines the problems of mathematical physics in 3-D with piece-wise coefficients are reduced with respect to one coordinate to 2-D problems. This procedure also allows to reduce the 2-D problems to 1-D problems and the solution of the approximated problemsa can be obtained analytically. In the case of constant piece-wise coefficients we obtain the exact discrete approximation of a steady-state 1-D boundary-value problem.

The solution of corresponding averaged 3-D initial-boundary value problem is also obtained numerically, using the discretization in space with the central diferences. The approximation of the 3-D nonstationary problem is based on the implicit finite-difference and alternating direction (ADI) methods. The numerical solution is compared with the analytical solution.

Keywords: special splines, averaging method, 3D problem, ADI method, analytical solution.

AMS Subject Classification: 65N06; 65N20; 65N40; 65N25; 34C55; 65N35.

1 Introduction

The task of sufficient accuracy numerical simulation of quick solution 3-D problems for mathematical physics in multi-layered media is important in the known areas of the applied sciences. With regard to the numerical analysis several numerical methods are known for solving 3-D problems: FEM, BEM, spectral

methods, multigrids and others methods. An example, in [6] a new template for stability analysis of numerical schemes for parabolic and pseudoparabolic problems with nonlocal conditions is given, in [10] efficient parallel algorithms of the OpenFOAM-based Parallel Solver for simulation of Electrical Power Cables are analysed. For simple engineering calculations two methods are applied [1], [2]: special finite difference scheme and conservative averaging method (CAM) by using special integral hyperbolic type splines with two parameters in every layer. We chose the CAM for engineering calculation and the solution of 3-D problem can be obtained analytically.
CAM by using integral parabolic type splines was developed by A. Buikis in his Doctoral Thesis [3] (in the Russian language) and in several papers [4], [11] etc. as a unified analytical (or analytically-numerical) approach to PDE with discontinuous coefficients. These methods were applied to create the mathematical simulation of the mass transfer 3-D initial-boundary-value problems for parabolic type partial differential equations of second order with piece-wise coefficients in multi-layered underground systems. Domains of a similar composition are examined using other mathematical methods in [5], [8].

In this Paper the special spline with two different functions, which interpolate middle integral values of piece-wise smooth function, is defined. These functions contain the independent solutions of corresponding homogeneous linear ODEs with parameters – characteristic values. Special hyperbolic and exponential type splines are developed. With the help of these splines the problems of mathematical physics in 3-D with piece-wise coefficients with respect to one coordinate are reduced to problems for system of PDEs in 2-D.
The solutions of corresponding 3-D initial-boundary value problem in one layer are obtained numerically, using the implicit alternating method by Duglas and Rackford (ADI) [7]. The 3-D problem in multi-layered domain is reduced to 2-D and 1-D problems, using special integral exponential - type splines. Every layer of these splines contain parameters, which can be selected in order to decrease the error of the solution. In the unlikely event if the parameters for the hyperbolic type spline tend to zero, we get the integral parabolic spline, obtained from A.Buikis.

2 Formulation of Problem

The process of diffusion and convection is considered in a 3-D parallelepiped

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

The domain Ω consist of multilayer medium.

We will consider the nonstationary 3-D problem for multi-layered piece-wise homogenous materials of N layers in the domain

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

where $H_i = z_i - z_{i-1}$ is the height of layer Ω_i, $z_0 = 0, z_N = L_z$.

We will find the distribution of mass transfer $c_i = c_i(x, y, z, t)$ in every layer Ω_i at the point $(x, y, z) \in \Omega_i$ and at the time t by solving the following 3-D initial-boundary value problem for partial differential equation of parabolic

type (PDE) [8]:

$$\begin{cases} \frac{\partial c_i}{\partial t} = \frac{\partial}{\partial x}(D_{ix}\frac{\partial c_i}{\partial x}) + r_{ix}\frac{\partial c_i}{\partial x} + \frac{\partial}{\partial y}(D_{iy}\frac{\partial c_i}{\partial y}) + r_{iy}\frac{\partial c_i}{\partial y} \\ \quad + \frac{\partial}{\partial z}(D_{iz}\frac{\partial c_i}{\partial z}) + r_{iz}\frac{\partial c_i}{\partial z} - a_{i0}^2 c_i + f_i, \\ x \in (0, L_x),\ y \in (0, L_y),\ z \in (z_{i-1}, z_i),\ t \in (0, t_f),\ i = \overline{1, N}, \\ \frac{\partial c_i(0,y,z,t)}{\partial x} = \frac{\partial c_i(x,0,z,t)}{\partial y} = 0, \\ D_{1z}\frac{\partial c_1(x,y,0,t)}{\partial z} - \beta_z(c_1(x,y,0,t) - c_{oz}(x,y)) = 0, \\ D_{ix}\frac{\partial c_i(L_x,y,z,t)}{\partial x} + \alpha_{ix}(c_i(L_x,y,z,t) - c_{iax}(y,z)) = 0,\ i = \overline{1, N}, \\ D_{iy}\frac{\partial c_i(x,L_y,z,t)}{\partial y} + \alpha_{iy}(c_i(x,L_y,z,t) - c_{iay}(x,z)) = 0,\ i = \overline{1, N}, \\ D_{Nz}\frac{\partial c_N(x,y,L_z,t)}{\partial z} + \alpha_z(c_N(x,y,L_z,t) - c_{az}(x,y)) = 0, \\ c_i(x,y,z_i,t) = c_{i+1}(x,y,z_i,t), \\ D_{iz}\frac{\partial c_i(x,y,z_i,t)}{\partial z} = D_{i+1,z}\frac{\partial c_{i+1}(x,y,z_1,t)}{\partial z},\ i = \overline{1, N-1} \\ c_i(x,y,z,0) = c_{i0}(x,y,z),\ i = \overline{1, N}, \end{cases} \tag{2.1}$$

where $c_i = c_i(x,y,z,t)$ are the solutions in every layer, $f_i = f_i(x,y,z,t)$ are the fixed sours functions, $D_{ix}, D_{iy}, D_{iz}, r_{ix}, r_{iy}, r_{iz}, a_{i0}$ are the constant coefficients, $\alpha_{ix}, \alpha_{iy}, \alpha_z, \beta_z$, $i = \overline{1, N}$ are the constant mass transfer coefficients in the third kind boundary conditions, $c_{az}, c_{iay}, c_{iax}, c_{oz}$ are the given concentration on the boundary, t_f is the final time, $c_{i0}(x,y,z)$ are the given initial concentration.

3 The averaging method in z-direction using the special integral spline with two fixed functions

By using the averaging method with respect to z with two fixed parametrical functions $f_{iz1}, f_{iz2}, i = \overline{1, N}$ we construct a spline

$$c_i(x,y,z,t) = c_{iz}(x,y,t) + m_{iz}(x,y,t)f_{iz1}(z - \overline{z_i}) + e_{iz}G_{iz}f_{iz2}(z - \overline{z_i}),$$

where $c_{iz}(x,y,t) = \frac{1}{H_i}\int_{z_{i-1}}^{z_i} c_i(x,y,z,t)dz$, $G_{iz} = H_i/D_{iz}$,

$$\int_{z_{i-1}}^{z_i} f_{iz1}\,dz = \int_{z_{i-1}}^{z_i} f_{iz2}\,dz = 0,\ \overline{z_i} = (z_{i-1} + z_i)/2,\ z \in [z_{i-1}, z_i],\ i = \overline{1, N}.$$

For example, using the exponential functions f_{iz1} and f_{iz2} can be defined in the following way:

$$f_{iz1} = \exp(a_{iz1}(z - \overline{z_i})) - \frac{2}{a_{iz1}H_i}\sinh(0.5a_{iz1}H_i),$$
$$f_{iz2} = \exp(a_{iz2}(z - \overline{z_i})) - \frac{2}{a_{iz2}H_i}\sinh(0.5a_{iz2}H_i),$$

where $a_{iz1} = -\frac{r_{iz}}{2D_{iz}} - \sqrt{\frac{r_{iz}^2}{4D_{iz}^2} + \frac{a_{i0}^2}{D_{iz}}}$, $a_{iz2} = -\frac{r_{iz}}{2D_{iz}} + \sqrt{\frac{r_{iz}^2}{4D_{iz}^2} + \frac{a_{i0}^2}{D_{iz}}}$.

We can determine the unknown functions $m_{iz}(x,y,t)$, $e_{iz}(x,y,t)$ from boundary conditions (2.1) in z-direction:

$$
\begin{aligned}
&1)\ m_{1z}a^m_{11} + G_{1z}e_{1z}a^m_{12} = \beta_z(c_{1z} - c_{0z}), \quad \text{for } z = 0,\\
&2)\ D_{Nz}(m_{Nz}f^{ap}_{Nz1} + G_{Nz}e_{Nz}f^{ap}_{Nz2}) + \alpha_z(c_{Nz} - c_{az}\\
&\qquad + m_{Nz}f^p_{Nz1} + e_{Nz}G_{Nz}f^p_{Nz2}) = 0, \quad \text{for } z = L_z,\\
&3)\ c_{iz} + m_{iz}f^p_{iz1} + e_{iz}G_{iz}f^p_{iz2} = c_{i+1,z} + m_{i+1,z}f^m_{i+1,z1} + e_{i+1,z}G_{i+1,z}f^m_{i+1,z2},\\
&\quad D_{iz}(m_{iz}f^{ap}_{iz1} + e_{iz}G_{iz}f^{ap}_{iz2}) = D_{i+1,z}(m_{i+1,z}f^{am}_{i+1,z1} + e_{i+1,z}G_{i+1,z}f^{am}_{i+1,z2}),\\
&\qquad \text{for } z = z_i, \quad i = \overline{1, N-1},
\end{aligned}
$$

where $f^m_{izk} = f_{izk}(-0.5H_i)$, $f^p_{izk} = f_{izk}(0.5H_i)$, $f^{am}_{izk} = \frac{\partial f_{izk}}{\partial z}(-0.5H_i)$, $f^{ap}_{izk} = \frac{\partial f_{izk}}{\partial z}(0.5H_i), k = 1;2$, $a^m_{11} = D_{1z}f^{am}_{1z1} - \beta_z f^m_{1z1}$, $a^m_{12} = D_{1z}f^{am}_{1z2} - \beta_z f^m_{1z2}$.

For determination of e_{iz}, from conditions on the contact lines $z = z_i$, $i = \overline{1, N-1}$, $z = z_{i-1}$, $i = \overline{2, N}$ by excluding $m_{i+1,z}$, $m_{i-1,z}$ and m_{iz} we obtain the following system of $N-2$ algebraic equations

$$
\begin{aligned}
a_{i,i}e_{iz} + a_{i,i+1}e_{i+1,z} + a_{i,i-1}e_{i-1,z} &= b_{i,i}c_{iz} + b_{i,i+1}c_{i+1,z}\\
&+ b_{i,i-1}c_{i-1,z}, \quad i = \overline{2, N-1},
\end{aligned}
$$

where $b_{i,i+1} = -c^m_{i1}$, $b_{i,i-1} = -c^p_{i1}$, $b_{i,i} = -(b_{i,i+1}+b_{i,i-1})$, $a_{i,i} = G_{iz}(b_{i,i+1}c^p_{i2}+b_{i,i-1}c^m_{i2})$, $a_{i,i+1} = G_{i+1,z}b_{i,i+1}c^p_{i3}$, $a_{i,i-1} = G_{i-1,z}c^p_{i1}c^m_{i3}$, $c^p_{i1} = f^p_{iz1} - \kappa_{iz1}f^m_{i+1,z1}$, $c^p_{i2} = f^p_{iz2} - \kappa_{iz2}f^m_{i+1,z1}$, $c^p_{i3} = \delta^m_{i+1,z}f^m_{i+1,z1} - f^m_{i+1,z2}$, $\kappa_{iz1} = \frac{D_{iz}f^{ap}_{iz1}}{D_{i+1,z}f^{am}_{i+1,z1}}$, $\kappa_{iz3} = \frac{D_{iz}f^{am}_{iz2}}{D_{i-1,z}f^{ap}_{i-1,z1}}$, $\kappa_{iz2} = \frac{D_{iz}f^{ap}_{iz2}}{D_{i+1,z}f^{am}_{i+1,z1}}$, $\delta^m_{i+1,z} = \frac{f^{am}_{i+1,z2}}{f^{am}_{i+1,z1}}$, $c^m_{i1} = \kappa^{-1}_{i-1,z1}f^p_{i-1,z1} - f^m_{iz1}$, $c^m_{i2} = f^m_{iz2} - \kappa_{i,z3}f^p_{i-1,z1}$, $c^m_{i3} = f^p_{i-1,z2} - \delta^p_{i-1,z}f^p_{i-1,z1}$, $\delta^p_{i-1,z} = f^{ap}_{i-1,z2}/f^{ap}_{i-1,z1}$.

From the boundary conditions at $z = 0, z = L_z$ and previous expressions for $i = 1$ and $i = N$ by excluding m_{1z}, m_{Nz} we get:

$$
\begin{aligned}
&a_{1,1}e_{1z} + a_{1,2}e_{2z} = b_{1,1}c_{1z} + b_{1,2}c_{2z} + b_{10}c_{0z},\\
&a_{N,N}e_{Nz} + a_{N,N-1}e_{N-1,z} = b_{N,N}c_{Nz} + b_{N,N-1}c_{N-1,z} + b_{N,0}c_{az},
\end{aligned}
$$

where $a_{1,1} = G_{1z}(c^p_{12}a^m_{11} - c^p_{11}a^m_{12})$, $a_{1,2} = G_{2,z}c^p_{13}a^m_{11}$, $b_{1,1} = -a^m_{11} - \beta_z c^p_{11}$, $b_{1,2} = a^m_{11}, b_{10} = \beta_z c^p_{11}$, $a_{N,N} = -G_{Nz}(c^m_{N1}a^p_{12} + c^m_{N2}a^p_{11})$, $a_{N,N-1} = G_{N-1,z}c^m_{N3}a^p_{11}$, $b_{N,N} = \alpha_z c^m_{N1} + a^p_{11}$, $b_{N,N-1} = -a^p_{11}$, $b_{N,0} = -\alpha_z c^m_{N1}$, $a^p_{11} = D_{Nz}f^{ap}_{Nz1} + \alpha_z f^p_{Nz1}$, $a^p_{12} = D_{Nz}f^{ap}_{Nz2} + \alpha_z f^p_{Nz2}$.

Using the obtained values $a_{i,j}, b_{i,j}$, $i,j = \overline{1, N}$ we can determine the 3-diagonal N-order matrices A^e_z, B^e_z with these elements, the N-order diagonal matrix B_0 with the elements $[b_{10}, 0, 0, ...0, b_{N,0}]$, the N-order vectors-column e_z, c_z with the elements e_{iz}, c_{iz} and the N-order vector-column c_0 with the elements $[c_{0z}, 0, 0, ...0, c_{az}]$. Then we have the system of N algebraic equations in the following vector form

$$
A^e_z e_z(x,y,t) = B^e_z c_z(x,y,t) + B_0 c_0(x,y). \tag{3.1}
$$

The matrix A^e_z is a diagonal dominant and we can write the unique solution in the form $e_z(x,y,t) = B^e_{1z}c_z(x,y,t) + B^e_{2z}c_0(x,y)$, where $B^e_{1z} = (A^e_z)^{-1}B^e_z, B^e_{2z} =$

$(A_z^e)^{-1}B_0$. Similarly we obtain $m_z(x,y,t) = B_{1z}^m c_z(x,y,t) + B_{2z}^m c_0(x,y)$, where $B_{1z}^m = B_z^m B_{1z}^e + C_z^m$, $B_{2z}^m = B_z^m B_{2z}^e + C_0^m$. Here B_z^m, C_z^m are the 2-diagonal N-order matrices with the elements $b_{1,1}^m = -\frac{G_{1z}a_{12}^m}{a_{11}^m}$, $b_{i,i-1}^m = -\frac{G_{i-1,z}c_{i3}^m}{c_{i1}^m}$, $b_{i,i}^m = \frac{G_{i,z}c_{i2}^m}{c_{i1}^m}$, $c_{1,1}^m = \frac{\beta_z}{a_{11}^m}$, $c_{i,i}^m = 1/c_{i1}^m, c_{i,i-1}^m = -1/c_{i1}^m$, C_0^m is the N-order diagonal matrix with the elements $[-\beta_z/a_{11}^m, 0, 0, ...0, 0]$.

We can determine the diagonal N-order matrices D_x, D_y, r_x, r_y, α_x, α_y, H_z^e, H_z^m, a_0^2 with the corresponding elements D_{ix}, D_{iy}, r_{ix}, r_{iy}, α_{ix}, α_{iy}, h_{iz}^e, h_{iz}^m, a_{i0}^2 and the N-order vectors-columns $f_z(x,y,t)$, $c_{ay}^v(x)$, $c_{ax}^v(y)$, $c_{z,0}$, c_z with the elements $f_{iz}(x,y,t)$, $c_{iay}^v(x)$, $c_{iax}^v(y)$, $c_{iz,0}(x,y)$, $c_{iz}(x,y,t)$, where $h_{iz}^e = \frac{G_{iz}}{H_i}(D_{iz}(f_{iz2}^{ap} - f_{iz2}^{am}) + r_{iz}(f_{iz2}^p - f_{iz2}^m))$, $h_{iz}^m = \frac{1}{H_i}(D_{iz}(f_{iz1}^{ap} - f_{iz1}^{am}) + r_{iz}(f_{iz1}^p - f_{iz1}^m))$, $f_{iz}(x,y,t) = \frac{1}{H_i}\int_{z_{i-1}}^{z_i} f_i(x,y,z,t)dz$, $c_{iax}^v(y) = \frac{1}{H_i}\int_{z_{i-1}}^{z_i} c_{iax}(y,z)dz$, $c_{iay}^v(x) = \frac{1}{H_i}\int_{z_{i-1}}^{z_i} c_{iay}(x,z)dz$, $c_{iz,0}(x,y) = \frac{1}{H_i}\int_{z_{i-1}}^{z_i} c_{i0}(x,y,z)dz$.

Then we have the new initial-boundary value 2D problem in following vector form:

$$\begin{cases} \frac{\partial c_z(x,y,t)}{\partial t} = \frac{\partial}{\partial x}(D_x\frac{\partial c_z(x,y,t)}{\partial x}) + r_x\frac{\partial c_z(x,y,t)}{\partial x} + \frac{\partial}{\partial y}(D_y\frac{\partial c_z(x,y,t)}{\partial y}) \\ \quad + r_y\frac{\partial c_z(x,y,t)}{\partial y} - a_0^2 c_z(x,y,t) + (Dh_z^e B_{1z}^e + Dh_z^m B_{1z}^m)c_z(x,y,t) \\ \quad + (Dh_z^e B_{2z}^e + Dh_z^m B_{2z}^m)c_0(x,y) + f_z(x,y,t), \\ \frac{\partial c_z(0,y,t)}{\partial x} = \frac{\partial c_z(x,0,t)}{\partial y} = 0, \\ D_x\frac{\partial c_z(L_x,y,t)}{\partial x} + \alpha_x(c_z(L_x,y,t) - c_{ax}^v(y)) = 0, \\ D_y\frac{\partial c_z(x,L_y,t)}{\partial y} + \alpha_y(c_z(x,L_y,t) - c_{ay}^v(x)) = 0, \\ c_z(x,y,0) = c_{z,0}(x,y), x \in (0,L_x), y \in (0,L_y), t \in (0,t_f). \end{cases} \tag{3.2}$$

4 The averaging method in y-direction

Using the averaging method with respect to y with two fixed parametrical functions f_{iy1}, f_{iy2}, $i = \overline{1,N}$:

$$c_{iz}(x,y,t) = c_{iy}(x,t) + m_{iy}(x,t)f_{iy1}(y - 0.5L_y) + e_{iy}(x,t)G_{iy}f_{iy2}(y - 0.5L_y),$$

where $c_{iy}(x,t) = \frac{1}{L_y}\int_0^{L_y} c_{iz}(x,y,t)dy$, $G_{iy} = \frac{L_y}{D_{iy}}$, $\int_0^{L_y} f_{iy1}dy = \int_0^{L_y} f_{iy2}dy = 0$, $i = \overline{1,N}$. For example, $f_{iy1} = \exp(a_{iy1}(y - 0.5L_y)) - \frac{2}{a_{iy1}L_y}\sinh(0.5a_{iy1}L_y)$, $f_{iy2} = \exp(a_{iy2}(y - 0.5L_y)) - \frac{2}{a_{iy2}L_y}\sinh(0.5a_{iy2}L_y)$, where $a_{iy1} = -\frac{r_{iy}}{2D_{iy}} - \sqrt{\frac{r_{iy}^2}{4D_{iy}^2} + \frac{k_{iy0}^2}{D_{iy}}}$, $a_{iy2} = -\frac{r_{iy}}{2D_{iy}} + \sqrt{\frac{r_{iy}^2}{4D_{iy}^2} + \frac{k_{iy0}^2}{D_{iy}}}$, $k_{iy0}^2 = a_{i0}^2 - a_{iy}$, $a_{iy} \le 0$ is the coefficient on c_{iz} in equations (3.2).

We can determine the unknown functions $m_{iy}(x,t), e_{iy}(x,t)$, from boundary conditions (3.2) in the following form:

$$D_{iy}(m_{iy}f_{iy1}^{ap} + e_{iy}G_{iy}f_{iy2}^{ap}) + \alpha_{iy}(m_{iy}f_{iy1}^p + e_{iy}G_{iy}f_{iy2}^p + c_{iy}(x,t) - c_{iay}^v(x)) = 0,$$
$$m_{iy}f_{iy1}^{am} + e_{iy}G_{iy}f_{iy2}^{am} = 0 \text{ or } e_{iy} = -b_{iy}(c_{iy}(x,t) - c_{iay}^v(x)),\ m_{iy} = -G_{iy}\kappa_{iy}^m e_{iy},$$

where $b_{iy} = \alpha_{iy}/(\alpha_{iy}G_{iy}(f^p_{iy2} - \kappa^m_{iy}f^p_{iy1}) + L_y(f^{ap}_{iy2} - \kappa^m_{iy}f^{ap}_{iy1}))$, $\kappa^m_{iy} = \frac{f^{am}_{iy2}}{f^{am}_{iy1}}$, $f^m_{iyk} = f_{iyk}(-0.5L_y)$, $f^p_{iyk} = f_{iyk}(0.5L_y)$, $f^{am}_{iyk} = \frac{\partial f_{iyk}}{\partial y}(-0.5L_y)$, $f^{ap}_{iyk} = \frac{\partial f_{iyk}}{\partial y}(0.5L_y)$, $k = 1, 2$.

Then the initial-boundary value problem (3.2) can be written in the following form

$$\begin{cases} \frac{\partial c_y(x,t)}{\partial t} = \frac{\partial}{\partial x}(D_x\frac{\partial c_y(x,t)}{\partial x}) + r_x\frac{\partial c_y(x,t)}{\partial x} - a_0^2 c_y(x,t) \\ \quad +(H^m_y B^m_y - H^e_y B^e_y)(c_y(x,t) - c^v_{ay}(x)) + (H^e_z B^e_{1z} + H^m_z B^m_{1z})c_y(x,t) \\ \quad +(H^e_z B^e_{2z} + H^m_z B^m_{2z})c^v_0(x) + f_y(x,t), \\ \frac{\partial c_y(0,t)}{\partial x} = 0, D_x\frac{\partial c_y(L_x,t)}{\partial x} + \alpha_x(c_y(L_x,t) - c^{vv}_{ax}) = 0, \\ c_y(x,0) = c_{y,0}(x), x \in (0, L_x), t \in (0, t_f), \end{cases} \tag{4.1}$$

where $H^e_y, H^m_y, B^e_y, B^m_y$ are the N-order diagonal matrices with the elements $h^e_{iy} = \frac{G_{iy}}{L_y}(D_{iy}(f^{ap}_{iy2} - f^{am}_{iy2}) + r_{iy}(f^p_{iy2} - f^m_{iy2}))$, $h^m_{iy} = \frac{1}{L_y}(D_{iy}(f^{ap}_{iy1} - f^{am}_{iy1}) + r_{iy}(f^p_{iy1} - f^m_{iy1}))$, $b^e_{iy} = b_{iy}, b^m_{iy} = G_{iy}\kappa^m_{iy}b_{iy}$, c_y, f_y are the N-order vectors-columns with the elements c_{iy}, f_{iy}, $c^v_0(x)$ is the N-order vector-column with two nonzero elements $c^v_{oz}(x)$, $c^v_{az}(x)$, $f_y(x,t) = \frac{1}{L_y}\int_0^{L_y} f_z(x,y,t)dy$, $c^v_{az}(x) = \frac{1}{L_y}\int_0^{L_y} c_{az}(x,y)dy$, $c^v_{oz}(x) = \frac{1}{L_y}\int_0^{L_y} c_{oz}(x,y)dy$, $c^{vv}_{ax} = \frac{1}{L_y}\int_0^{L_y} c^v_{ax}(y)dy$, $c_{y,0}(x) = \frac{1}{L_y}\int_0^{L_y} c_{z,0}(x,y)dy$.

5 The averaging method in x-direction

It is also possible to do the averaging with respect to x coordinate:

$$c_{ix}(t) = \frac{1}{L_x}\int_0^{L_x} c_{iy}(x,t)dx, \quad c_{iy}(x,t) = c_{ix}(t) + m_{ix}(t)f_{ix1}(x - 0.5L_x)$$
$$+ e_{ix}(t)G_{ix}f_{ix2}(x - 0.5L_x), \quad \int_0^{L_x} f_{ix1}dy = \int_0^{L_x} f_{ix2}dy = 0,$$

with the unknown functions $m_{ix}(t), e_{ix}(t)$. For example,

$$f_{ix1} = \exp(a_{ix1}(x - 0.5L_x)) - \frac{2}{a_{ix1}L_x}\sinh(0.5a_{ix1}L_x),$$
$$f_{ix2} = \exp(a_{ix2}(x - 0.5L_x)) - \frac{2}{a_{ix2}L_x}\sinh(0.5a_{ix2}L_x),$$

where $a_{ix1} = -\frac{r_{ix}}{2D_{ix}} - \sqrt{\frac{r^2_{ix}}{4D^2_{ix}} + \frac{k^2_{ix0}}{D_{ix}}}$, $a_{ix2} = -\frac{r_{ix}}{2D_{ix}} + \sqrt{\frac{r^2_{ix}}{4D^2_{ix}} + \frac{k^2_{ix0}}{D_{ix}}}$, $k^2_{ix0} = a^2_{i0} - a_{ix}$, $a_{ix} \le 0$ is the coefficient depending on c_{iy} in (4.1).

We can determine these functions from boundary conditions (4.1) in the following form:

$$D_{ix}(m_{ix}f^{ap}_{ix1} + e_{ix}G_{ix}f^{ap}_{ix2}) + \alpha_x(m_{ix}f^p_{ix1} + e_{ix}G_{ix}f^p_{ix2} + c_{ix}(t) - c^{vv}_{iax}) = 0,$$
$$m_{ix}f^{am}_{ix1} + e_{ix}G_{ix}f^{am}_{ix2} = 0 \text{ or } e_{ix} = -b_{ix}(c_{ix}(t) - c^{vv}_{iax}), \quad m_{ix} = -G_{ix}\kappa^m_{ix}e_{ix},$$

where $b_{ix} = \alpha_{ix}/(\alpha_{ix}G_{ix}(f^p_{ix2} - \kappa^m_{ix}f^p_{ix1}) + L_x(f^{ap}_{ix2} - \kappa^m_{ix}f^{ap}_{ix1}))$, $\kappa^m_{ix} = \frac{f^{am}_{ix2}}{f^{am}_{ix1}}$, $G_{ix} = \frac{L_x}{D_{ix}}$, $f^m_{ixk} = f_{ixk}(-0.5L_x)$, $f^p_{ixk} = f_{ixk}(0.5L_x)$, $f^{am}_{ixk} = \frac{\partial f_{ixk}}{\partial x}(-0.5L_x)$, $f^{ap}_{ixk} = \frac{\partial f_{ixk}}{\partial x}(0.5L_x)$, $k = 1, 2$.

Then the initial-boundary value problem (4.1) can be written in the following form:

$$\begin{cases} \frac{\partial c_x(t)}{\partial t} = (H^m_y B^m_y - H^e_y B^e_y)(c_x(t) - c^{vv}_{ay}) + (H^e_z B^e_{1z} + H^m_z B^m_{1z})c_x(t) - a_0^2 c_x(t) \\ \quad + (H^e_z B^e_{2z} + H^m_z B^m_{2z})c^{vv}_0 + (H^m_x B^m_x - H^e_x B^e_x)(c_x(t) - c^{vv}_{ax}) + f_x(t), \\ c_x(0) = c_{x,0}, \quad t \in (0, t_f), \end{cases} \tag{5.1}$$

where $H^e_x, H^m_x, B^e_x, B^m_x$ are the N-order diagonal matrices with the elements $h^e_{ix} = \frac{G_{ix}}{L_x}(D_{ix}(f^{ap}_{ix2} - f^{am}_{ix2}) + r_{ix}(f^p_{ix2} - f^m_{ix2}))$, $h^m_{ix} = \frac{1}{L_x}(D_{ix}(f^{ap}_{ix1} - f^{am}_{ix1}) + r_{ix}(f^p_{ix1} - f^m_{ix1}))$, $b^e_{ix} = b_{ix}, b^m_{ix} = G_{ix}\kappa^m_{ix}b_{ix}$, c_x, f_x are the N-order vectors-columns with elements c_{ix}, f_{ix}, c^{vv}_0, are the N-order vector-column with two nonzero elements c^{vv}_{oz}, c^{vv}_{az},

$$f_x(t) = \frac{1}{L_x}\int_0^{L_x} f_y(x,t)\,dx, \quad c_{x,0} = \frac{1}{L_x}\int_0^{L_x} c_{y,0}(x)\,dx,$$
$$c^{vv}_{az} = \frac{1}{L_x}\int_0^{L_x} c^v_{az}(x)\,dx, \quad c^{vv}_{0z} = \frac{1}{L_x}\int_0^{L_x} c^v_{0z}(x)\,dx.$$

Therefore from (5.1) we have the initial value problem for the system of N ODEs of the first order. The solutions for this system can be obtained with classical methods.

For the averaged stationary solution (f_x is a constant vector) we also get the analytical solution in the form

$$c_x = (H_{x,y,z})^{-1}(-f_x + g),$$

where $H_{x,y,z} = H^e_z B^e_{1z} + H^m_z B^m_{1z} + H^m_y B^m_y - H^e_y B^e_y + H^m_x B^m_x - H^e_x B^e_x - a_0^2$, is the N-order matrix and $g = (H^m_x B^m_x - H^e_x B^e_x)c^{vv}_{ax} + (H^m_y B^m_y - H^e_y B^e_y)c^{vv}_{ay} - (H^e_z B^e_{2z} + H^m_z B^m_{2z})c^{vv}_0$ is the N-order vector-column.

6 CAM for solving 1-D multi-layer diffusion problem with the hyperbolic type integral spline

For solving (2.1) without convection $r_{ix} = r_{iy} = r_{iz} = 0$ we consider hyperbolic functions in the z-direction with parameters $a_{iz1}, a_{iz2}, i = \overline{1, N}$:

$$f_{iz1} = \frac{0.5H_i \sinh(a_{iz1}(z - \overline{z_i}))}{\sinh(0.5a_{iz1}H_i)}, \quad f_{iz2} = (0.25\frac{\sinh^2(a_{iz2}(z - \overline{z_i}))}{\sinh^2(0.5a_{iz2}H_i} - A_{i0z}),$$

where $A_{i0z} = 0.25\frac{(sinh(a_{iz2}H_i))/(a_{iz2}H_i)-1}{cosh(a_{iz2}H_i)-1} \in [0, 1/12]$. We see that the parameters a_{iz1}, a_{iz2} tend to zero when the limit is the integral parabolic spline [4], because $A_{i0z} \to \frac{1}{12}$ as $f_{iz1} = (z - \overline{z_i})$, $f_{iz2} = \frac{(z-\overline{z_i})^2}{H_i^2} - \frac{1}{12}$. We also see

that $f^m_{iz1} = -0.5H_i$, $f^p_{iz1} = 0.5H_i$, $f^m_{iz2} = f^p_{iz2} = A_{i1z}$, $f^{am}_{iz1} = f^{ap}_{iz1} = d_{iz1}$, $f^{am}_{iz2} = -d_{iz2}$, $f^{ap}_{iz2} = d_{iz2}$, where $A_{i1z} = 0.25 - A_{i0z} \in [1/6, 1/4]$, $A_{i1z} \to \frac{1}{6}$, $d_{iz1} = 0.5H_i a_{iz1} \coth(0.5a_{iz1}H_i) \to 1$, $d_{iz2} = 0.5H_i a_{iz2} \coth(0.5a_{iz2}H_i) \to 1$, if $a_{iz1}, a_{iz2} \to 0$.

It is possible to show that this spline for $a_{iz1} = \sqrt{a^2_{i0}/D_{iz}}, a_{iz2} = 0.5a_{iz1}$ integrate exactly the following 1D boundary-value problem:

$$\begin{cases} \frac{\partial}{\partial z}(D_{iz}\frac{\partial c_i(z)}{\partial z}) - a^2_{i0}c_i(z) + F_i = 0, \quad z \in (z_{i-1}, z_i),\ i = \overline{1, N}, \\ D_{1z}\frac{\partial c_1(0)}{\partial z} - \beta_z(c_1(0) - C_0) = 0, \\ D_{Nz}\frac{\partial c_N(L_z)}{\partial z} + \alpha_z(c_N(L_z) - C_a) = 0, \\ c_i(z_i) = c_{i+1}(z_i), D_{iz}\frac{\partial c_i(z_i)}{\partial z} = D_{i+1,z}\frac{\partial c_{i+1}(z_1)}{\partial z}, \quad i = \overline{1, N-1}, \end{cases} \tag{6.1}$$

where F_i, C_0, C_a are constant parameter.

Table 1. The maximal error δ and averaged values c^v_{an}-exact, c^v_{ap} - approx)

α_z	β_z	a_1	a_2	δ	c^v_{ap}	c^v_{an}
2	1	0	0	0.092	0.769	0.792
-	-	0.5	0.5	0.084	0.802	-
-	-	1.0	1.0	0.062	0.785	-
-	-	1.4	1.4	0.050	0.791	-
-	-	1.5	1.5	0.050	0.802	-
-	-	b	b/2	0.0	0.792	0.792
2	0	0	0	0.339	0.672	0.808
-	-	1.3	1.3	0.243	0.727	-
-	-	2.0	2.0	0.134	0.791	-
-	-	2.5	2.5	0.088	0.843	-
-	-	2.3	2.3	0.081	0.822	-
-	-	b	b/2	0.0	0.808	0.808
20	0	0	0	0.339	0.672	0.809
-	-	2.3	2.3	0.081	0.823	-
-	-	b	b/2	0.0	0.809	0.809

Example 1. We consider the 1-D problem (6.1) with one layer (N=1) in the following form:

$$\begin{cases} \frac{\partial}{\partial z}(\frac{\partial c(z)}{\partial z}) - b^2c(z) + f_0 = 0, \quad z \in (0, L_z), \\ D_z\frac{\partial c(0)}{\partial z} - \beta_z(c(0) - C_0) = 0, D_z\frac{\partial c(L_z)}{\partial z} + \alpha_z(c(L_z) - C_a) = 0, \end{cases}$$

where $b^2 = a^2_0/D_z, f_0 = F/D_z$. Therefore the exact solution is

$$c(z) = P_1\sinh(bz) + P_2\cosh(bz) + f_0/b^2,$$

where the constants

$$P_1 = \beta_z\big(P_2 + f_0/b^2/D_z b - C_0\big), \quad P_2 = \alpha_z\big(C_a - f_0/b^2\big) + \beta\big(C_0 - f_0/b^2\big) \times \big(\cosh(bL_z) + \alpha_z\sinh(bL_z)/(bD_z)\big)/\big(\cosh(bL_z)(\alpha_z + \beta_z) + \sinh(bL_z)(bD_z + \alpha_z\beta_z/(bD_z))\big).$$

The averaged values are $c^v = L_z^{-1}\int_0^{L_z} c(z)dz = \frac{1}{L_z b}(P_1(\cosh(bL_z) - 1) + P_2\sinh(bL_z)) + f_0/b^2$.

This form of solution was also applied to discreate approximation $c(z_j), z_j = jh, h = \frac{L_z}{N}, j = \overline{0,N}$ by using the exact finite difference scheme (FDS) from N. Bahvalov [1]. For comparison we use the averaged method with respect to z for hyperbolic type integral spline.

The Table 1 shows the numerical results for $F = 0, L_z = 1, L_x = 1, L_y = 1, C_0 = 0.3, C_a = 2.0, D_z = 10^{-3}$, $D_x = D_y = 3 \cdot 10^{-4}$, $b = 2.4335$. The maximal error δ and averaged values are presented, the dependence on $a_1 = a_{z1}$, $a_2 = a_{z2}$, α_z, β_z ($a_1 = a_2 = 0$ for parabolic spline) is investigated.

Figures 1, 2 represent the solutions $c(z)$ for $N = 20$, $\alpha_z = 20$, $\beta_z = 0$, $a_1 = a_2 = 2.3$ and for $a_1 = b, a_2 = b/2$, respectively. Note that for $a_1 = a_2$ and FDS we get $\delta = 0.0222$, and for $a_1 = b$, $a_2 = b/2$ we get $\delta = 0$. For $L_z = 3, F = 0.1, b = 2.4335$ follows: $c^v_{ap} = 23.14$, $c^v_{an} = 16.87$, $\delta = 6.27$ (for parabolic spline), $c^v_{ap} = 16.87$, $c^v_{an} = 16.87$, $\delta = 0$ (for hyperbolic type spline with $a_1 = b, a_2 = b/2$).

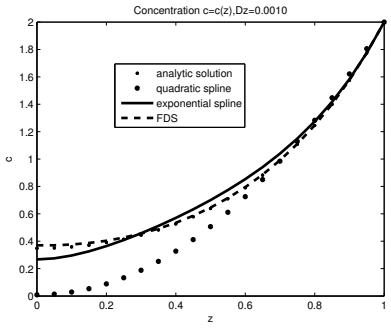

Figure 1. One layer solution c(z) for $L_z = 1, \alpha_z = 20, \beta_z = 0, a_1 = a_2 = 2.3$

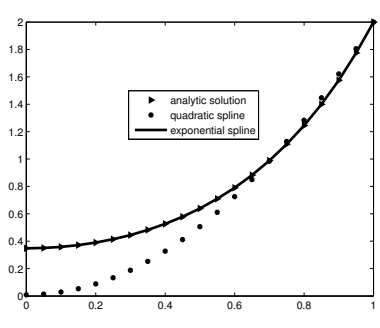

Figure 2. One layer solution $c(z)$ for $L_z = 3, D_{1z} = 10e-03, D_{2z} = 10e-04, a_2 = a_1/2$

Figures 3, 4 represent the functions f_{1z}, f_{2z} for the hyperbolic spline depending on parameters $a_1 = a_2 \in [0, 25]$, and for the parabolic spline $a_1 = a_2 = 0$. For the spline with 2 parameters $a_1 = b, a_2 = b/2$ we have the exact solution for all values of parameters $L_z, F, b, D_z, C_0, C_a, \alpha, \beta$.

7 CAM for solving 1-D multi-layer mass transfer problem with the exponential type integral spline

It is possible to show that the integral spline integrates the exact following 1D boundary-value problem in N layers:

$$\begin{cases} \frac{\partial}{\partial z}(D_{iz}\frac{\partial c_i(z)}{\partial z}) + r_{iz}\frac{\partial c_i(z)}{\partial z} - a_{i0}^2 c_i(z) + F_i = 0, z \in (z_{i-1}, z_i), i = \overline{1,N}, \\ D_{1z}\frac{\partial c_1(0)}{\partial z} - \beta_z(c_1(0) - C_0) = 0, \\ D_{Nz}\frac{\partial c_N(L_z)}{\partial z} + \alpha_z(c_N(L_z) - C_a) = 0, \\ c_i(z_i) = c_{i+1}(z_i), D_{iz}\frac{\partial c_i(z_i)}{\partial z} = D_{i+1,z}\frac{\partial c_{i+1}(z_1)}{\partial z}, i = \overline{1,N-1}, \end{cases} \tag{7.1}$$

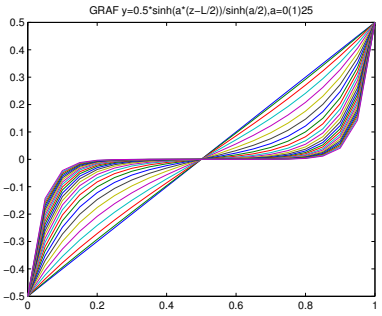

Figure 3. Values of functions f_{1z} for hyperbolic spline with $a_1 = a_2 \in [0, 25]$

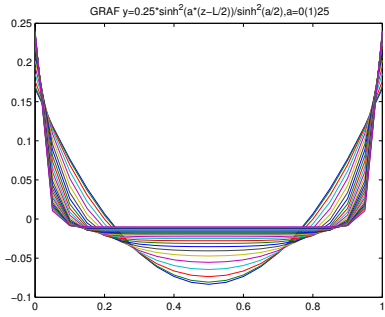

Figure 4. Values of functions f_{2z} for hyperbolic spline with $a_1 = a_2 \in [0, 25]$

where F_i, C_0, C_a are constant parameters (see Section 10 ($N = 5$ and $N = 10$)).

Using the averaging in z-direction (3.1,3.2) we have the averaged value c_z^v for the solution $c_i(z)$ of boundary-value problem (7.1) in the following matrix form:

$$c_z^v = (a_{02} - H_z^e B_{1z}^e - H_z^m B_{1z}^m)^{-1}\big((H_z^e B_{2z}^e + H_z^m B_{2z}^m)c_0 + F\big),$$

where the elements on the diagonal of N-order matrices H_z^e, H_z^m are $h_{iz}^e = \frac{2G_z}{H_i}(D_{iz}a_{iz2} + r_{iz})\sinh(0.5a_{iz2}H_i)$ and $h_{iz}^m = \frac{2}{H_i}(D_{iz}a_{iz1} + r_{iz})\sinh(0.5a_{iz1}H_i)$.

The spline-solution is defined as:

$$c(z) = c_z^v + F_{z1}m_z + G_z F_{z2}e_z$$

with N-order diagonal matrices F_{z1}, F_{z2}, G_z. Similarly the exact analytical solution of (7.1) can be obtained.

For two layers (N=2) by $L_z = 3, H_1 = 1.8, H_2 = 1.2, D_1 = 10^{-3}$, $D_2 = 10^{-4}$, $\alpha_1 = 10^6, \beta_1 = 10^3, C_0 = 0.3$, $C_a = 3.0$, $r_1 = -0.01$, $r_2 = 0.01, F_1 = 0.001, F_2 = 0.001$, we have the following numerical results (see Figure 5): the maximal error – $2 \cdot 10^{-7}$ (exponential spline), 0.6045 (parabolic spline), the averaged values $c_1^v = 0.3332$, $c_2^v = 0.8391$ (exact and exponential splines), $c_1^v = 0.3662$, $c_2^v = 0.8055$ (parabolic spline). Figure 6 represents how function f_{1z1} for exponential spline is depending on the parameter $a1_{1z} \in [-5, 5]$.

8 CAM for solving 3-D diffusion problem in one layer with the exponential type integral spline

For averaging (2.1) in one layer ($\overline{z_1} = L_z/2$) we consider exponential functions following in the z-direction. From boundary conditions the system of two algebraic equations follows

$$\begin{cases} b_{11}m_z + b_{12}e_z = \beta_z(c_z - c_{0z}), \\ b_{21}m_z + b_{22}e_z = -\alpha_z(c_z - c_{az}), \end{cases}$$

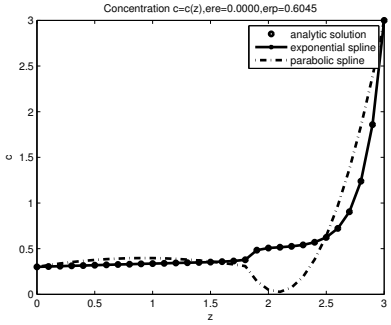

Figure 5. Two layers solutions for $L_z = 3, D_{1z} = 10e-03, D_{2z} = 10e-04$

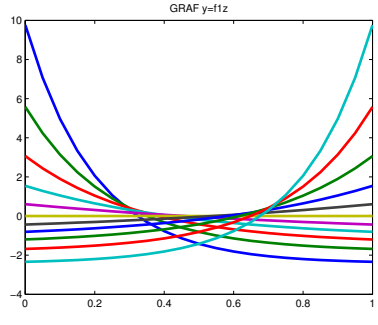

Figure 6. Values of functions f_{1z1} for exponential spline, $a1_{1z} \in [-5(1)5]$

where $b_{11} = D_z f_{z1}^{am} - \beta_z f_{z1}^{m}$, $b_{21} = D_z f_{z1}^{ap} + \alpha_z f_{z1}^{p}$, $b_{12} = L_z f_{z2}^{am} - G_z \beta_z f_{z2}^{m}$, $b_{22} = L_z f_{z2}^{ap} + G_z \alpha_z f_{z2}^{p}$. The solution is given in the form

$$m_z = a_m c_z - b_m c_{az} - c_m c_{0z}, \quad e_z = -a_e c_z - b_e c_{az} + c_e c_{0z},$$

where $a_m = (\beta_z b_{22} + \alpha_z b_{12})/d, b_m = \alpha_z b_{12}/d, c_m = \beta_z b_{22}/d$, $a_e = (\alpha_z b_{11} + \beta_z b_{21})/d, b_e = \alpha_z b_{11}/d$, $c_e = \beta_z b_{21}/d$, $d = b_{11} b_{22} - b_{12} b_{21}$.

The new 2D initial-boundary value problem is in the form

$$\begin{cases} \frac{\partial c_z(x,y,t)}{\partial t} = \frac{\partial}{\partial x}(D_x \frac{\partial c_z(x,y,t)}{\partial x}) + r_x \frac{\partial c_z(x,y,t)}{\partial x} \\ \quad + \frac{\partial}{\partial y}(D_y \frac{\partial c_z(x,y,t)}{\partial y}) + r_y \frac{\partial c_z(x,y,t)}{\partial y} + (g_z - a_0^2) c_{iz}(x,y,t) \\ \quad + a_z c_{az} + b_z c_{0z} + f_z(x,y,t), \\ \frac{\partial c_z(0,y,t)}{\partial x} = \frac{\partial c_z(x,0,t)}{\partial y} = 0, \\ D_x \frac{\partial c_z(L_x,y,t)}{\partial x} + \alpha_x (c_z(L_x,y,t) - c_{ax}^v(y)) = 0, \\ D_y \frac{\partial c_z(x,L_y,t)}{\partial y} + \alpha_y (c_z(x,L_y,t) - c_{ay}^v(x)) = 0, \\ c_z(x,y,0) = c_{z,0}(x,y), \quad x \in (0,L_x), \ y \in (0,L_y), \ t \in (0,t_f), \end{cases}$$

where $g_z = b_1 a_m - b_2 G_z a_e \le 0, a_z = -b_1 b_m + b_1 G_z b_e, b_z = -b_1 c_m + b_2 G_z c_e$, $b_1 = \frac{2}{L_z} \sinh(a_{z1} L_z/2)(D_z a_{z1} + r_z), b_2 = \frac{2}{L_z} \sinh(a_{z2} L_z/2)(D_z a_{z2} + r_z)$.

For averaging in the y-direction we use the following parameters:

$$a_{y1} = -\frac{r_y}{2D_y} - \sqrt{\frac{r_y^2}{4D_y^2} + \frac{(a_0^2 - g_z)}{D_y}}, \quad a_{y2} = -\frac{r_y}{2D_y} + \sqrt{\frac{r_y^2}{4D_y^2} + \frac{(a_0^2 - g_z)}{D_y}}.$$

We see that $f_{yk}^{p} = d_{kpy}$, $f_{yk}^{am} = a_{yk} \exp(-0.5 a_{yk} L_y)$, $f_{yk}^{ap} = a_{yk} \exp(0.5 a_{yk} L_y)$, $f_{yk}^{p} = \exp(0.5 a_{yk} L_y) - \frac{2}{a_{yk} L_y} \sinh(0.5 a_{yk} L_y)$, $k = 1, 2$.

It follows from boundary conditions that

$$m_y = -e_y G_y \kappa_y, \quad e_y = -b_y (c_y - c_{ay}^v),$$

where $\kappa_y = f_{y2}^{am}/f_{y1}^{am}$, $b_y = \alpha_y / \big(L_y (f_{y2}^{ap} - \kappa_y f_{y1}^{ap}) + \alpha_y G_y (f_{y2}^{p} - \kappa_y f_{y1}^{p})\big)$.

The new 1D initial-boundary value problem is in the form

$$\begin{cases} \frac{\partial c_y(x,t)}{\partial t} = \frac{\partial}{\partial x}(D_x \frac{\partial c_y(x,t)}{\partial x}) + r_x \frac{\partial c_z(x,t)}{\partial x} \\ \quad +(g_z - a_0^2 - b_y g_y) c_y(x,t) + a_z c_{az}^v + b_z c_{0z}^v + b_y g_y c_{ay}^v + f_y(x,t), \\ \frac{\partial c_y(0,t)}{\partial x} = 0, D_x \frac{\partial c_y(L_x,t)}{\partial x} + \alpha_x (c_y(L_x,t) - c_{ax}^{vv}) = 0, \\ c_y(x,0) = c_{y,0}(x), \quad x \in (0, L_x), \ \ t \in (0, t_f), \end{cases}$$

where $g_y = f_{y2}^{ap} - \kappa_y f_{y1}^{ap} + \frac{2r_y}{D_y}(-\kappa_y \sinh(a_{y1} L_y/2) + \sinh(a_{y2} L_y/2)) \geq 0$.

For averaging in the x-direction we use $a_{x1} = -\frac{r_x}{2D_x} - \sqrt{\frac{r_x^2}{4D_x^2} + \frac{(a_0^2 - g_z + b_y g_y)}{D_x}}$, $a_{x2} = -\frac{r_x}{2D_x} + \sqrt{\frac{r_x^2}{4D_x^2} + \frac{(a_0^2 - g_z + b_y g_y)}{D_x}}$. Then we get $f_{xk}^p = \exp(0.5 a k_x L_x) - \frac{2}{a k_x L_x} \sinh(0.5 a k_x L_x)$, $f_{xk}^{am} = a k_x \exp(-0.5 a k_x L_x)$, $f_{xk}^{ap} = a k_x \exp(0.5 a k_x L_x)$, $k = 1, 2$.

From boundary conditions it follows that

$$m_x = -e_x G_x \kappa_x, \quad e_x = -b_x (c_x - c_{ax}^{vv}),$$

where $\kappa_x = f_{x2}^{am}/f_{x1}^{am}$, $b_x = \alpha_x / (L_x (f_{x2}^{ap} - \kappa_x f_{x1}^{ap}) + \alpha_x G_x (f_{x2}^p - \kappa_x f_{x1}^p))$.

We have the following initial value problem for ODEs of the first order:

$$\begin{cases} \frac{\partial c_x(t)}{\partial t} = (g_z - a_0^2 - b_y g_y - b_x g_x) c_x(t) \\ \quad + a_z c_{az}^{vv} + b_z c_{0z}^{vv} + b_y g_y c_{ay}^{vv} + b_x g_x c_{ax}^{vv} + f_x(t), \\ c_x(0) = c_{x,0}, \quad t \in (0, t_f), \end{cases}$$

where $g_x = f_{x2}^{ap} - \kappa_x f_{x1}^{ap} + \frac{2r_x}{D_x}(-\kappa_x \sinh(a_{x1} L_x/2) + \sinh(a_{x2} L_x/2)) \geq 0$.

For the stationary solution we get

$$c_x = \frac{a_z c_{az}^{vv} + b_z c_{0z}^{vv} + b_y g_y c_{ay}^{vv} + b_x g_x c_{ax}^{vv} + f_x}{-g_z + a_0^2 + b_y g_y + b_x g_x}.$$

Then we have the stationary 3D solution in following analytical form:
$c_y(x) = c_x + m_x f_{x1} + e_x G_x f_{x2}$, $e_y(x) = -b_y (c_y(x) - c_{ay}^v)$, $m_y(x) = -e_y(x) G_y \kappa_y$,
$c_z(x,y) = c_y(x) + m_y(x) f_{y1}(y) + e_y(x) G_y f_{y2}(y)$,
$e_z(x,y) = -a_e c_z(x,y) - b_e c_{az} + c_e c_{0z}$, $m_z(x,y) = a_m c_z(x,y) - b_m c_{az} - c_m c_{0z}$,
$c(x,y,z) = c_z(x,y) + m_z(x,y) f_{z1}(z) + e_z(x,y) G_z f_{z2}(z)$.

9 The numerical approximations with ADI method for the 3-D problem in one layer

We use a uniform space grid $(K+1) \times (\tilde{N}+1) \times (M+1)$:

$$\big\{(z_k, y_i, x_j), \ \ z_k = (k-1)h_z, \ \ y_i = (i-1)h_y, \ \ x_j = (j-1)h_x, \ \ i = \overline{1, \tilde{N}+1}, \\ j = \overline{1, M+1}, \ \ k = \overline{1, K+1}, \ \ K\, h_z = L_z, \tilde{N}, \ \ h_y = L_y, \ \ M\, h_x = L_x\big\}.$$

For the time t we use the discrete grid $t_n = n\tau, n = 0, 1, \ldots$. Subscripts (k, i, j, n) refer to z, y, x, t indices with the grid spacing, and for the approximation of function $c(z, y, x, t)$ we get a grid function $U_{k,i,j}^n \approx c(z_k, y_i, x_j, t_n)$.

For solving 3D problem (2.1) we use the discrete approximation

$$(U^{n+1}_{k,i,j} - U^n_{k,i,j})/\tau = (\Lambda_z + \Lambda_y + \Lambda_x)U^{n+1}_{k,i,j} + f^n_{k,i,j}, \quad n \geq 0,$$

$k = \overline{1, K+1}$, $i = \overline{1, \tilde{N}+1}$, $j = \overline{1, M+1}$ and ADI method by Douglas and Rachford [7,9]:

$$\begin{cases} (U^{n+1/3}_{k,i,j} - U^n_{k,i,j})/\tau = \Lambda_z U^{n+1/3}_{k,i,j} + \Lambda_y U^n_{k,i,j} + \Lambda_x U^n_{i,j} + f^n_{i,j}, \\ k = \overline{2, K}, \quad i = \overline{2, \tilde{N}}, \quad j = \overline{2, M}, \\ (U^{n+2/3}_{k,i,j} - U^{n+1/3}_{k,i,j})/\tau = \Lambda_y (U^{n+2/3}_{k,i,j} - U^n_{k,i,j}), \\ k = \overline{1, K+1}, \quad i = \overline{2, \tilde{N}}, \quad j = \overline{1, M+1}, \\ (U^{n+1}_{k,i,j} - U^{n+2/3}_{k,i,j})/\tau = \Lambda_x (U^{n+1}_{k,i,j} - U^n_{k,i,j}), \\ k = \overline{1, K+1}, \quad i = \overline{1, \tilde{N}+1}, \quad j = \overline{2, M}. \end{cases} \tag{9.1}$$

After elimating the unknowns at fractional time moments $t_{n+1/3}, t_{n+2/3}$ we obtain the previous discrete problem with approximation error $O(\tau^2)$. Here $\Lambda_x, \Lambda_y, \Lambda_z$ are the difference operators, approximated the differential operators

$$\frac{\partial}{\partial x}\Big(D_x \frac{\partial c(z,y,x,t)}{\partial x}\Big) + r_x \frac{\partial c(z,y,x,t)}{\partial x}, \quad \frac{\partial}{\partial y}\Big(D_y \frac{\partial c(z,y,x,t)}{\partial y}\Big) + r_y \frac{\partial c(z,y,x,t)}{\partial y},$$

$$\frac{\partial}{\partial z}\Big(D_z \frac{\partial c(z,y,x,t)}{\partial z}\Big) + r_z \frac{\partial c(z,y,x,t)}{\partial z} - a_0^2 c(z,y,x,t)$$

and boundary conditions with central differences, $f^n_{k,i,j} = f_z(z_k, y_i, x_j, t_n)$. The approximation is monotonous if $h_x \leq \frac{2D_x}{|r_x|}$, $h_y \leq \frac{2D_y}{|r_y|}$, $h_z \leq \frac{2D_z}{|r_z|}$. For solving $U^{n+1/3}$, $U^{n+2/3}$ and U^{n+1} we use Thomas algorithm in z, y and x directions respectively.

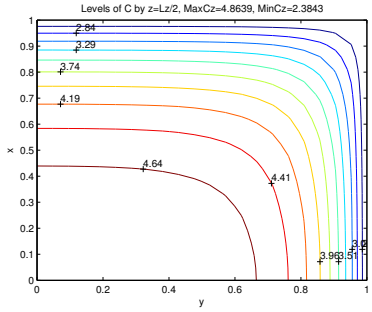

Figure 7. Levels of averaged concentration $c(x, y, L_z/2)$

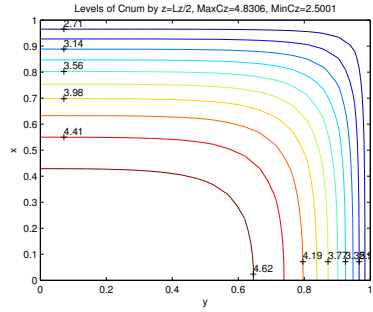

Figure 8. Levels of numerical concentration $c(x, y, L_z/2)$

10 Numerical results

The numerical results are obtained for $K = 19, \tilde{N} = M = 21$, $L_z = 3$, $L_x = L_y = 1$, $\alpha_z = 20, \beta_z = 10, \alpha_x = \alpha_y = 2, c_{az} = 4, c_{0z} = 1.3, c_{ax} = c_{ay} = 2.5$,

$D_x = D_y = 3 \cdot 10^{-3}$, $D_z = 10^{-2}, r_z = 0.01, r_x = 0.001, r_y = -0.001, f = 0.1, a_0 = 0.1$. We have following numerical values: $g_z = -0.069, b_y g_y = 0.0129, b_x g_x = 0.0281, a1_z = -10.1, a2_z = 0.1, a1_y = -3.73, a2_y = 7.06, a1_x = -7.45, a2_x = 3.73$.

For using the ADI method for the initial condition the stationary averaged solution $c_z(x, y, z)$ is selected. We have the stationary solution with $\tau = 1$, $t_f = 300$, then the maximal error is 10^{-8}, the maximal value of $c(x, y, z)$ is 5.29 for averaged method, 5.16 for ADI method (see Figures 7–10).

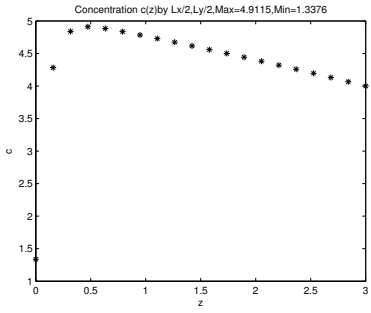

Figure 9. Averaged and numerical concentration $c(L_x/2, L_y/2, z)$

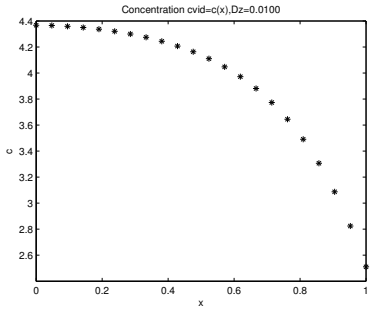

Figure 10. Averaged concentration $c_x(x)$

Depending on the number of grid points $(K, \tilde{N}, M)$ we have the following maximal values of the solution for ADI method: 5.1616 ($K = 19$, $M = \tilde{N} = 21$), 5.1587 ($K = 29$, $M = \tilde{N} = 31$).

Figure 11 shows the graphics of functions $c_i(z)$ (7.1) in 5 uniform layers $(N = 5, H_i = 0.6, L_z = 3, \beta_z = \alpha_z = 10, C_0 = 0.3, C_a = 2)$ for $D_{iz} = [0.01; 2; 0.03; 4; 0.05]$, r_{iz}=[0.1; 0.2; 0.3; 0.4; 0.5], F_i=[0.04; 0.08; 0.12; 0.16; 0.20], $a^2_{i0} = [0.1; 0.2; 0.3; 0.4; 0.5]$. In Figure 12 the parameters remain the same, only the source term F_i has the opposite sign.

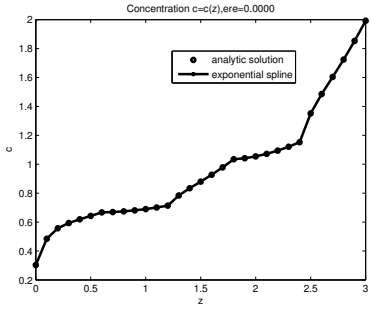

Figure 11. Function $c(z)$ for a positive source F(N=5)

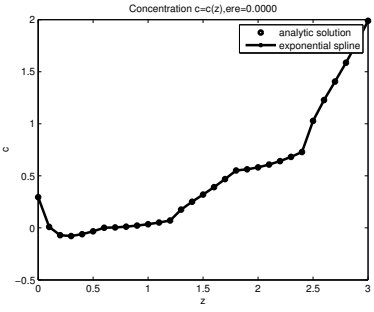

Figure 12. Function $c(z)$ for a negative source F(N=5)

Figure 13 shows the graphics of functions $c_i(z)$ (7.1) in 10 uniform layers

$(N = 10, H_i = 0.6, L_z = 6, \beta_z = \alpha_z = 10, C_0 = 0.3, C_a = 2)$ for

$$D_{iz} = [0.01; 2; 0.03; 4; 0.05; 0.01; 2; 0.03; 4; 0.05],$$
$$r_{iz} = [0.1; 0.2; 0.3; 0.4; 0.5; 0.1; 0.2; 0.3; 0.4; 0.5],$$
$$F_i = [0.04; 0.08; 0.12; 0.16; 0.20; 0.04; 0.08; 0.12; 0.16; 0.20],$$
$$a_{i0}^2 = [0.1; 0.2; 0.3; 0.4; 0.5; 0.1; 0.2; 0.3; 0.4; 0.5].$$

In Figure 14 the parameters remain the same as in Figure 13, but the source term F_i has an opposite sign.

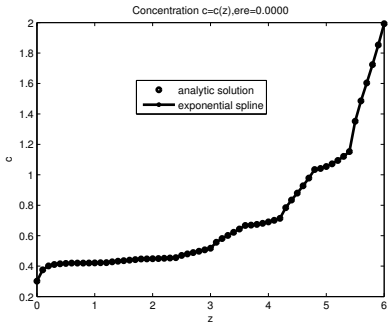

Figure 13. Function $c(z)$ for a positive source F(N=10)

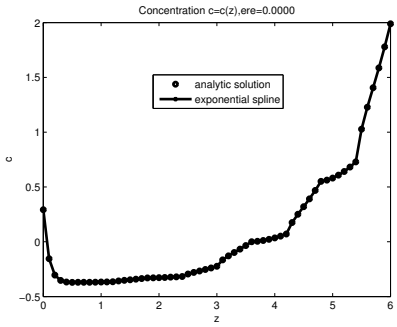

Figure 14. Function $c(z)$ for a negative source F(N=10)

11 Conclusions

The 3-D mass transfer problem in multi-layered domain is reduced to 2-D and 1-D problems using the special integral parabolic , hyperbolic and exponential type splines. These splines are obtained from the general spline with two fixed functions. The parameters of these functions are the characteristic values for the corresponding homogeneous ODEs of second order in fixed direction. These parameters are the best parameters for minimal error.

The 1-D differential and discrete problems are solved analytically. For hyperbolic spline the best parameter for minimal error is calculated.

The solutions for the corresponding averaged non-stationary 3-D initial-boundary value problem are obtained numerically using alternating-direction implicit (ADI) method proposed by Douglas and Rachford.

The stationary numerical solution is compared with the analytical solution. The max absolute value of difference between corresponding numerical and averaged data was 1–2 percent.

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