

**ON THE MATHEMATICAL MODELLING OF THE DIFFUSION
EQUATION WITH PIECEWISE CONSTANT COEFFICIENTS
IN A MULTI-LAYERED DOMAIN**

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Abstract: In this paper a 2-D stationary boundary value-problem for the diffusion equation with piecewise constant coefficients in a multi-layered domain is considered. Homogeneous boundary conditions of the first kind (BC) or periodic boundary conditions (PBC) are considered in the x direction. An analytical method for solving the problem of the above type is developed. This method is compared with the averaging (AV) method (using integral parabolic splines) and finite difference methods (using second-order finite difference schemes (FDS) for the space discretization in the x direction) and the finite difference scheme with exact spectrum (FDSES).

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1. Introduction

We consider a 2-D stationary boundary-value-problem for the diffusion equation with piecewise constant coefficients in a multi-layered domain. In the x direction we have homogeneous boundary condition of the first kind (BC) or periodic boundary conditions (PBC).

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We define the finite difference scheme with exact spectrum (FDSES) (see [5], [4], [7]) using the finite difference matrix A in the form $A = WDW^T$ (W, D are matrices, containing finite difference eigenvectors and eigenvalues), where the elements of the diagonal matrix D are replaced with the first K eigenvalues of the second order differential operator ($K = N - 1$ for BCs of the first kind, $K = N$ for PBCs, where $N + 1$ is a number of grid points in a uniform grid). Also we consider the method of lines and Fourier methods for solving the corresponding problems with homogeneous BCs and PBCs.

A. Buikis (see [1], [2]) developed averaging methods. These methods can be applied on mathematical simulation of the mass transfer process in multi-layered underground systems. In order to solve this problem, it is necessary to solve the 3-D initial-boundary-value problems for parabolic second order partial differential equations with piece-wise parameters in a multilayer domain. Special splines which interpolate middle integral values of a piece-wise smooth function allow to reduce the 3-D mathematical physics problem with piece-wise coefficients to 2-D problems for the system of equations.

H.Kalis (see [3]) developed an effective finite-difference method for solving the problem of the above type. This method may be considered as a generalization of the finite volumes method for layered systems. This procedure allows to reduce the 2-D problem to the system of 1-D problems.

All these methods are applied on the problem. The solutions are obtained analytically and numerically.

2. The Mathematical Model

The process of diffusion is considered in the 2-D domain

$$\Omega = \{(x, y) : 0 \leq x \leq l, 0 \leq y \leq L\}.$$

The domain Ω consists of a multi-layered medium. We consider the 2-D stationary problem from the linear diffusion theory for multi-layered piece-wise homogeneous materials with M layers in the following form:

$$\Omega_j = \{(x, y) : x \in (0, l), y \in (y_{j-1}, y_j)\}, \quad i = \overline{1, M},$$

where $y_j - y_{j-1} = h_j$ is the height of the corresponding layer Ω_j , $y_0 = 0, y_M = L$. The distribution of the concentrations $u_j = u_j(x, y)$ in each layer Ω_j at each point $(x, y) \in \Omega_j$ will be found by solving the following PDEs:

$$k_j \partial^2 u_j / \partial x^2 + k_j \partial^2 u_j / \partial y^2 + f_j(x, y) = 0, \quad (1)$$

where k_j are constant diffusion coefficients, $u_j = u_j(x, y)$ – concentration functions in each layer, $f_j(x, y)$ – fixed source functions.

The values u_j and the flux functions $k_j \partial u_j / \partial y$ should be continuous on the contact lines between the layers $y = y_j, j = \overline{1, M-1}$:

$$\begin{aligned} u_j(x, y_j) &= u_{j+1}(x, y_j), \\ k_j \partial u_j(x, y_j) / \partial y &= k_{j+1} \partial u_{j+1}(x, y_j) / \partial y. \end{aligned} \tag{2}$$

We assume that the layered material is bounded above and below with the plane surfaces $y = 0, y = L$ with fixed BCs of the third kind in the following form:

$$\begin{aligned} \gamma_1 k_1 \partial u_1(x, 0) / \partial y - \alpha_1 (u_1(x, 0) - T_1(x)) &= 0, \\ \gamma_2 k_M \partial u_M(x, L) / \partial y + \alpha_2 (u_M(x, L) - T_2(x)) &= 0, \end{aligned} \tag{3}$$

where $\gamma_1^2 + \alpha_1^2 \neq 0, \gamma_2^2 + \alpha_2^2 \neq 0, T_1, T_2$ are given functions. For $\gamma_1 = \gamma_2 = 0$ we have BCs of the first kind. We shall consider two forms of fixed BCs in the x, y directions:

1) the periodic BCs at $x = 0, x = l$:

$$u_j(0, y) = u_j(l, y), \quad \partial u_j(0, y) / \partial x = \partial u_j(l, y) / \partial x, \tag{4}$$

2) the homogeneous BCs of the first kind:

$$u_j(0, y) = u_j(l, y) = 0, \quad j = \overline{1, M}. \tag{5}$$

3. Analytical Solution with Fourier Methods

For the analytical solution of the problem (1)-(5) we consider Fourier series methods:

1. For the BC (5):

$$\begin{aligned} u_j(x, y) &= \sum_{k=1}^{\infty} a_{j,k}(y) X_k(x), \\ f_j(x, y) &= \sum_{k=1}^{\infty} b_{j,k}(y) X_k(x), \quad T_m(x) = \sum_{k=1}^{\infty} c_{m,k} X_k(x), \end{aligned}$$

where $m = 1; 2$,

$$X_k(x) = \sqrt{\frac{2}{l}} \sin \frac{k\pi x}{l}$$

are the orthonormal eigenfunctions;

$$(X_k, X_m) = \int_0^l X_k(x)X_m(x)dx = \delta_{k,m}$$

with the eigenvalues $\lambda_k = (\frac{k\pi}{l})^2$, $-\frac{d^2X_k(x)}{dx^2} = \lambda_k X_k(x)$, $X_k(0) = X_k(l) = 0$, $b_{j,k}(y) = (f_j, X_k)$, $c_{m,k} = (T_m, X_k)$, $m = 1; 2$, and $\delta_{k,m}$ is the Kronecker delta.

2. For the BC (4):

$$u_j(x, y) = \sum_{k=-\infty}^{\infty} a_{j,k}(y)X_k(x),$$

$$f_j(x, y) = \sum_{k=-\infty}^{\infty} b_{j,k}(y)X_k(x), \quad T_m(x) = \sum_{k=-\infty}^{\infty} c_{m,k}X_k(x),$$

where $m = 1; 2$,

$$X_k(x) = \sqrt{\frac{1}{l}} \exp(2\pi i k x / l),$$

$$X_k^*(x) = \sqrt{\frac{1}{l}} \exp(-2\pi i k x / l),$$

$i = \sqrt{-1}$ are the biorthonormal complex eigenvectors

$$(X_k, X_m^*) = \int_0^l X_k(x)X_m^*(x)dx = \delta_{k,m}$$

with the eigenvalues $\lambda_k = (\frac{2k\pi}{l})^2$, $-\frac{d^2X_k(x)}{dx^2} = \lambda_k X_k(x)$, $X_k(0) = X_k(l)$, $X_k'(0) = X_k'(l)$, $b_{j,k}(y) = (f_j, X_k^*)$, $c_{m,k} = (T_m, X_k^*)$.

We can also consider *the real Fourier series*. For a periodic function $g(x)$ with the period l we have the complex Fourier series

$$g(x) = \sum_{k=-\infty}^{\infty} a_k X_k(x),$$

where $a_k = (g, X_k^*) = \int_0^l g(x)X_k^*(x)dx$ or $g(x) = \sum_{k=1}^{\infty} (a_k X_k(x) + a_{-k} X_{-k}) + \frac{a_0}{\sqrt{l}}$.

Taking into account that $X_{-k}(x) = X_k^*(x)$, $\lambda_{-k} = \lambda_k$, $a_k = \frac{a_k + a_{-k}}{2} + \frac{a_k - a_{-k}}{2}$, $a_{-k} = \frac{a_k + a_{-k}}{2} - \frac{a_k - a_{-k}}{2}$, $a_k^{(1)} = \frac{a_k + a_{-k}}{\sqrt{l}}$, $a_k^{(2)} = \frac{i(a_k + a_{-k})}{\sqrt{l}}$ we have the real Fourier series in the following form:

$$g(x) = \sum_{k=1}^{\infty} (a_k^{(1)} \cos \frac{2\pi kx}{l} + a_k^{(2)} \sin \frac{2\pi kx}{l}) + \frac{a_0^{(1)}}{2},$$

where

$$a_k^{(1)} = \frac{1}{\sqrt{l}}(g, X_k + X_k^*) = \frac{2}{l} \int_0^l g(x) \cos \frac{2\pi kx}{l} dx,$$

$$a_k^{(2)} = \frac{i}{\sqrt{l}}(g, X_k^* - X_k) = \frac{2}{l} \int_0^l g(x) \sin \frac{2\pi kx}{l} dx.$$

Using the previous transformations the following expressions can be obtained:

$$u_j(x, y) = \sum_{k=1}^{\infty} (a_{j,k}^{(1)}(y) \cos \frac{2\pi kx}{l} + a_{j,k}^{(2)}(y) \sin \frac{2\pi kx}{l}) + \frac{a_{j,0}^{(1)}(y)}{2},$$

$$f_j(x, y) = \sum_{k=1}^{\infty} (b_{j,k}^{(1)}(y) \cos \frac{2\pi kx}{l} + b_{j,k}^{(2)}(y) \sin \frac{2\pi kx}{l}) + \frac{b_{j,0}^{(1)}(y)}{2},$$

$$T_m(x) = \sum_{k=1}^{\infty} (c_{m,k}^{(1)} \cos \frac{2\pi kx}{l} + c_{m,k}^{(2)} \sin \frac{2\pi kx}{l}) + \frac{c_{m,0}^{(1)}}{2}, \quad m = 1; 2,$$

where

$$b_{j,k}^{(1)}(y) = \frac{2}{l} \int_0^l f_j(x, y) \cos \frac{2\pi kx}{l} dx,$$

$$b_{j,k}^{(2)}(y) = \frac{2}{l} \int_0^l f_j(x, y) \sin \frac{2\pi kx}{l} dx,$$

$$c_{m,k}^{(1)} = \frac{2}{l} \int_0^l T_m(x) \cos \frac{2\pi kx}{l} dx,$$

$$c_{m,k}^{(2)} = \frac{2}{l} \int_0^l T_m(x) \sin \frac{2\pi kx}{l} dx, \quad m = 1; 2.$$

For the Fourier coefficients $a_{j,k}(y)$ or $a_{j,k}^{(1)}(y), a_{j,k}^{(2)}(y)$ we have the following boundary-value-problem for the system of ODEs:

$$\begin{cases} -k_j \lambda_k a_{j,k}(y) + k_j a''_{j,k}(y) = -b_{j,k}(y), y \in (y_{j-1}, y_j), j = \overline{1, M} \\ a_{j,k}(y_j) = a_{j+1,k}(y_j), k_j a'_{j,k}(y_j) = k_{j+1} a'_{j+1,k}(y_j), j = \overline{1, M-1} \\ \gamma_1 k_1 a'_{1,k}(0) - \alpha_1 (a_{1,k}(0) - c_{1,k}) = 0 \\ \gamma_2 k_M a'_{M,k}(L) + \alpha_2 (a_{M,k}(L) - c_{2,k}) = 0, \end{cases} \tag{6}$$

where $a''_{j,k}(y) = \frac{d^2 a_{j,k}(y)}{d^2 y}, a'_{j,k}(y) = \frac{da_{j,k}(y)}{dy}$.

The general solution of the system (6) is as follows:

$$a_{j,k}(y) = C_{j,k} \sinh(\sqrt{\lambda_k}(y - y_{j-1})) + B_{j,k} \cosh(\sqrt{\lambda_k}(y - y_{j-1})) - \frac{1}{k_j \sqrt{\lambda_k}} \int_{y_{j-1}}^y \sinh(\sqrt{\lambda_k}(y - t)) b_{j,k}(t) dt, \tag{7}$$

where the constants $C_{j,k}, B_{j,k}$ can be determined from the following system of algebraic equations:

$$\begin{aligned} k_{j+1} C_{j+1,k} &= k_j (C_{j,k} ch_{j,k} + B_{j,k} sh_{j,k}) - \frac{1}{\sqrt{\lambda_k}} IC_{j,k}, \\ B_{j+1,k} &= C_{j,k} sh_{j,k} + B_{j,k} ch_{j,k} - \frac{1}{k_j \sqrt{\lambda_k}} IS_{j,k}, \quad j = \overline{1, M-1}, \\ \gamma_1 k_1 C_{1,k} \sqrt{\lambda_k} - \alpha_1 (B_{1,k} - c_{1,k}) &= 0, \end{aligned}$$

$$\begin{aligned} \gamma_2 (k_M \sqrt{\lambda_k} (C_{M,k} ch_{M,k} + B_{M,k} sh_{M,k}) - IC_{M,k}) \\ + \alpha_2 (C_{M,k} sh_{M,k} + B_{M,k} ch_{M,k} - \frac{1}{k_M \sqrt{\lambda_k}} IS_{M,k}) - c_{2,k} &= 0. \end{aligned}$$

Here $sh_{j,k} = \sinh(\sqrt{\lambda_k} h_j), ch_{j,k} = \cosh(\sqrt{\lambda_k} h_j),$

$$IS_{j,k} = \int_{y_{j-1}}^{y_j} \sinh(\sqrt{\lambda_k}(y_j - t)) b_{j,k}(t) dt, IC_{j,k} = \int_{y_{j-1}}^{y_j} \cosh(\sqrt{\lambda_k}(y_j - t)) b_{j,k}(t) dt.$$

4. The AV-Method with Quadratic Splines

The equations (1) are averaged along the heights h_j of the corresponding layers Ω_j with quadratic integral splines in the following form [1]:

$$u_j(x, y) = U_j(x) + m_j(x)(y - \bar{y}_j) + e_j(x)G_j((y - \bar{y}_j)^2/h_j^2 - 1/12), \quad (8)$$

where $G_j = h_j/k_j, \bar{y}_j = (y_{j-1} + y_j)/2, y \in [y_{j-1}, y_j], m_j, e_j, U_j$ are the unknown coefficients of the spline-functions,

$$U_j(x) = h_j^{-1} \int_{y_{j-1}}^{y_j} u_j(x, y) dy$$

are the averaged values of $u_j, j = \overline{1, M}$.

After averaging the system (1) along each layer Ω_j , we obtain the system of M ODEs:

$$k_j \frac{d^2 U_j(x)}{dx^2} + 2h_j^{-1} e_j(x) + F(x) = 0, \quad (9)$$

where $F_j = h_j^{-1} \int_{y_{j-1}}^{y_j} f_j(x, y) dy$ are the average values of $f_j, j = \overline{1, M}$.

Using the boundary conditions (4),(5) and excluding the coefficients m_j we obtain the following system of linear algebraic equations [2]:

$$A_j e_{j-1} + (A_j + B_j + 1) e_j + B_j e_{j+1} = a_j (U_{j+1} - U_j) - b_j (U_j - U_{j-1}), \quad j = \overline{1, M}, \quad (10)$$

where

$$e_0 = e_{M+1} = 0, A_j = G_{j-1}/(G_j + G_{j-1}), b_j = 3/(G_j + G_{j-1}) = a_{j-1}, j = \overline{2, M},$$

$$B_j = G_{j+1}/(G_j + G_{j+1}), a_j = 3/(G_j + G_{j+1}), j = \overline{1, M-1},$$

$$a_M = 1.5\alpha_2/(\gamma_2 + \alpha_2 G_M/2), b_1 = 1.5\alpha_1/(\gamma_1 + \alpha_1 G_1/2),$$

$$A_1 = \gamma_1/(\gamma_1 + \alpha_1 G_1/2), B_M = \gamma_2/(\gamma_2 + \alpha_2 G_M/2),$$

$$U_0 = T_1, U_{M+1} = T_2.$$

5. The Finite Difference Approximation

For solving 2-D problems we consider an uniform grid in the x -direction $x_k = kh, Nh = l, k = \overline{0, N}$. We can rewrite the PDEs (1) in the following vector form:

$$-k_j Av_j(y) + k_j v_j''(y) + g_j(y) = 0, j = \overline{1, M}, \tag{11}$$

where $v_j(y), g_j(y)$ are the column vectors with the elements

$$v_{j,k} \approx u_j(x_k, y), g_{j,k} = f_j(x_k, y), \quad k = \overline{1, K},$$

A are the finite difference 3-diagonal K -order matrices in following forms:

- 1) for the BCs of the first kind, $K = N - 1$,

$$A = \frac{1}{h^2} \begin{pmatrix} 2 & -1 & 0 & \dots & 0 & 0 & 0 \\ -1 & 2 & -1 & \dots & 0 & 0 & 0 \\ \dots & \dots & \dots & \dots & \dots & \dots & \dots \\ 0 & 0 & 0 & \dots & -1 & 2 & -1 \\ 0 & 0 & 0 & \dots & 0 & -1 & 2 \end{pmatrix}$$

- 2) for the periodic BCs, $K = N$,

$$A = \frac{1}{h^2} \begin{pmatrix} 2 & -1 & 0 & \dots & 0 & 0 & -1 \\ -1 & 2 & -1 & \dots & 0 & 0 & 0 \\ \dots & \dots & \dots & \dots & \dots & \dots & \dots \\ 0 & 0 & 0 & \dots & -1 & 2 & -1 \\ -1 & 0 & 0 & \dots & 0 & -1 & 2 \end{pmatrix}$$

This circulant matrix can be determined using only the first row

$$A = \frac{1}{h^2} [2 \ -1 \ 0 \ \dots \ 0 \ 0 \ -1],$$

see [6].

From the conditions (2, 3) follows, that:

$$\begin{cases} v_j(y_j) = v_{j+1}(y_j), \\ k_j v_j'(y_j) = k_{j+1} v_{j+1}'(y_j), \\ \gamma_1 k_1 v_1(0) - \alpha_1 (v_1(0) - \mathbf{T}_1) = 0, \\ \gamma_2 k_M v_M(L) + \alpha_2 (v_M(L) - \mathbf{T}_2) = 0, \end{cases} \tag{12}$$

where $\mathbf{T}_1, \mathbf{T}_2$ are the K order column vectors with the elements $T_1(x_k), T_2(x_k), k = \overline{1, K}$.

The calculation of the circulant matrix (matrix inversion and multiplication) can be done by using the first row of the matrix, see [6].

6. The Finite Difference Schemes Solution

The solution of the corresponding discrete spectral problem $Aw^k = \mu_k w^k$ is:

1. For the BCs the of first kind we have $k = \overline{1, N-1}$, the orthonormal eigenvectors

$$(w^k, w^m) = \sum_{j=1}^{N-1} w_j^k w_j^m = \delta_{k,m},$$

$$w_j^k = \sqrt{\frac{2}{N}} \sin \frac{\pi j k}{N},$$

$j, k = \overline{1, N-1}$ (the elements of the symmetric matrix W), the eigenvalues $\mu_k = \frac{4}{h^2} \sin^2 \frac{k\pi}{2N}$ (the elements of the diagonal matrix D);

2. For the periodic BCs we have $k = \overline{1, N}$, the biorthonormal complex eigenvectors

$$(w^k, w_*^m) = \sum_{j=1}^N w_j^k w_{*j}^m = \delta_{k,m},$$

$$w_j^k = \sqrt{\frac{1}{N}} \exp(2\pi i k j / N), w_{*j}^k = \sqrt{\frac{1}{N}} \exp(-2\pi i k j / N), i = \sqrt{-1}$$

(the elements of the complex matrices W, W_*), the eigenvalues $\mu_k = \frac{4}{h^2} \sin^2 \frac{k\pi}{N}$ (the elements of the diagonal matrix D).

Further, we shall consider *discrete real Fourier series*. For the N -order vector g and the elements $g_s, s = \overline{1, N}$ we have the following complex expression $g = \sum_{k=1}^N a_k w^k$, where

$$a_k = (g, w_*^k) = \sum_{s=1}^N g_s w_s^k$$

or

$$g = \sum_{k=1}^{*\bar{N}} (a_k w^k + a_{N-k} w^{N-k}) + \frac{a_N}{\sqrt{N}},$$

$$w^{N-k} = w_*^k, \quad w_*^{N-k} = w^k, \quad \mu_{N-k} = \mu_k,$$

$$\sum_{k=1}^{*\bar{N}} a_k = \sum_{k=1}^{\bar{N}-1} a_k + a_{\bar{N}}/2, \quad \bar{N} = N/2.$$

Using the expressions

$$a_k = \frac{a_k + a_{N-k}}{2} + \frac{a_k - a_{N-k}}{2},$$

$$a_{N-k} = \frac{a_k + a_{N-k}}{2} - \frac{a_k - a_{N-k}}{2}, \quad a_k^{(1)} = \frac{a_k + a_{N-k}}{\sqrt{N}}, a_k^{(2)} = \frac{i(a_k - a_{N-k})}{\sqrt{N}}$$

we have the discrete real Fourier series in the following form:

$$g_s = \sum_{k=1}^{*\bar{N}} (a_k^{(1)} \cos \frac{2\pi ks}{N} + a_k^{(2)} \sin \frac{2\pi ks}{N}) + \frac{a_0^{(1)}}{2}, \quad a_N = a_0,$$

where

$$a_k^{(1)} = \frac{1}{\sqrt{N}}(g, w_*^k + w_*^{N-k}) = \frac{2}{N} \sum_{s=1}^N g_s \cos \frac{2\pi ks}{N},$$

$$a_k^{(2)} = \frac{i}{\sqrt{N}}(g, w_*^k - w_*^{N-k}) = \frac{2}{N} \sum_{s=1}^N g_s \sin \frac{2\pi ks}{N}.$$

For the PBCs we consider the finite difference approximation of the second-order for the derivative $u''(x_k)$ in the uniform $p + 1$ point stencil

$$(x_{k-p/2}, \dots, x_{k-1}, x_k, x_{k+1}, \dots, x_{k+p/2}).$$

We consider the approximation of the $O(h^p)$ order in following form:

$$u''(x_k) = \frac{1}{h^2} \sum_{m=-p/2}^{p/2} C_m u(x_{k-m}) + E_p \frac{h^p u^{(p+2)}(\xi)}{(p+2)!}, \quad x_{k-p/2} < \xi < x_{k+p/2}.$$

For $m = 0$ follows the equation $C_0 = -2 \sum_{m=1}^{p/2} C_m$. The other coefficients $C_m (m > 0)$ can be determined from the system of linear algebraic equations. Solving this system we obtain the following coefficients:

- 1) $p = 2 : C_1 = 1, C_0 = -2, E_2 = -2,$
- 2) $p = 4 : C_1 = \frac{4}{3}, C_2 = -\frac{1}{12}, C_0 = -\frac{5}{2}, E_4 = 8,$
- 3) $p = 6 : C_1 = \frac{3}{2}, C_2 = -\frac{3}{20}, C_3 = \frac{1}{90}, C_0 = -\frac{49}{18}, E_4 = -72,$
- 4) $p = 8 : C_1 = \frac{8}{5}, C_2 = -\frac{1}{5}, C_3 = \frac{8}{315}, C_4 = -\frac{1}{560}, C_0 = -\frac{205}{72}, E_8 = 1152.$

In this case A is a circulant matrix in the form:

$$A = \frac{1}{h^2} [C_0, C_1, \dots, C_{p/2}, 0, \dots, 0, C_{p/2}, C_{p/2-1}, \dots, C_2, C_1]$$

and it has the following eigenvalues ($k = \overline{1, N}$):

- 1) $p = 2 : \mu_k = \frac{4}{h^2} \sin^2(\pi k/N),$
- 2) $p = 4 : \mu_k = \frac{4}{h^2} (\sin^2(\pi k/N) + \frac{1}{3} \sin^4(\pi k/N)),$
- 3) $p = 6 : \mu_k = \frac{4}{h^2} (\sin^2(\pi k/N) + \frac{1}{3} \sin^4(\pi k/N) + \frac{8}{45} \sin^6(\pi k/N)),$
- 4) $p = 8 : \mu_k = \frac{4}{h^2} (\sin^2(\pi k/N) + \frac{1}{3} \sin^4(\pi k/N) + \frac{8}{45} \sin^6(\pi k/N) + \frac{4}{35} \sin^8(\pi k/N)).$

In the matrix form we have (for the BCs of the first kind $W_* = W$):

$$AW = WD, \quad WW_* = E, \quad W^{-1} = W_*, \quad A = WDW_*,$$

where the elements of the diagonal matrix D are $d_k = \mu_k$.

Using the transformation $\bar{v}_j(y) = W^T v_j(y)$ ($W^T = W_*$ for the periodic BCs, $W^T = W$ for the BCs of the first kind) in (11) we obtain the following system of ODEs:

$$-k_j D \bar{v}_j(y) + k_j \bar{v}_j''(y) + \bar{g}_j(y) = 0, \quad j = \overline{1, M}, \tag{13}$$

or:

$$-k_j d_k \bar{v}_{j,k}(y) + k_j \bar{v}_{j,k}''(y) + \bar{g}_{j,k}(y) = 0, \quad j = \overline{1, M}, \quad k = \overline{1, K}, \tag{14}$$

where $\bar{g}_j = W^T g_j$, d_k are the elements of the matrix D , $\bar{v}_{j,k}, \bar{g}_{j,k}$ are the elements of the vectors \bar{v}_j, \bar{g}_j .

For (13) we have the following conditions:

$$\begin{cases} \bar{v}_{j,k}(y_j) = \bar{v}_{j+1,k}(y_j), k_j \bar{v}'_{j,k}(y_j) = k_{j+1} \bar{v}'_{j+1,k}(y_j), \quad j = \overline{1, M-1} \\ \gamma_1 k_1 \bar{v}'_{1,k}(0) - \alpha_1 (\bar{v}_{1,k}(0) - \bar{c}_{1,k}) = 0 \\ \gamma_2 k_M \bar{v}'_{M,k}(L) + \alpha_2 (\bar{v}_{M,k}(L) - \bar{c}_{2,k}) = 0, \quad k = \overline{1, K}, \end{cases} \tag{15}$$

where $\bar{c}_{1,k}, \bar{c}_{2,k}$ are the elements of the vectors $W^T T_1, W^T T_2$. The solution of (14, 15) is the form (7), where $a_{j,k}, \lambda_k, c_{1,k}, c_{2,k}$ are replaced with $\bar{v}_{j,k}, d_k, \bar{c}_{1,k}, \bar{c}_{2,k}$.

For the *finite difference scheme with exact spectrum* (FDSES) the matrix A is represented in the Jordan normal form $A = WDW^T$ and the diagonal matrix D contains the first K eigenvalues $d_k = \lambda_k, k = \overline{1, K}$ of the differential operator $(-\frac{\partial^2}{\partial x^2})$. The eigenvectors remain the same.

For the FDSES with the periodic BCs the elements of the matrix D are replaced in following way:

- 1) $d_k = \lambda_k$ for $k = \overline{1, N_2}$, where $N_2 = N/2$.
- 2) $d_k = \lambda_{N-k}$ for $k = \overline{N_2, N-1}, d_N = 0$.

We can solve the equation (11), using the discrete Fourier series in the following form:

$$v_j(y) = \sum_{k=1}^K a_{j,k} w^k, g_j(y) = \sum_{k=1}^K b_{j,k} w^k,$$

$$\mathbf{T}_m = \sum_{k=1}^K c_{m,k} w^k,$$

where $b_{j,k}(y) = (g_j(y), w_*^k)$, $c_{m,k}(y) = (\mathbf{T}_m, w_*^k)$, $m = 1; 2$, $K = N$ for the PBCs, $K = N - 1$, $w_*^k = w^k$ for the BCs of the first kind.

For the PBCs we can use the real argument expressions:

$$v_{j,s}(y) = \sum_{k=1}^{*\bar{N}} (a_{j,k}^{(1)}(y) \cos \frac{2\pi ks}{N} + a_{j,k}^{(2)}(y) \sin \frac{2\pi ks}{N}) + a_{j,0}^{(1)}(y)/2,$$

$$g_{j,s}(y) = \sum_{k=1}^{*\bar{N}} (b_{j,k}^{(1)}(y) \cos \frac{2\pi ks}{N} + b_{j,k}^{(2)}(y) \sin \frac{2\pi ks}{N}) + b_{j,0}^{(1)}(y)/2,$$

$$T_m(x_s) = \sum_{k=1}^{*\bar{N}} (c_{m,k}^{(1)} \cos \frac{2\pi ks}{N} + c_{m,k}^{(2)} \sin \frac{2\pi ks}{N}) + c_{m,0}^{(1)}/2,$$

where $b_{j,k}^{(1)}(y) = \frac{2}{N} \sum_{s=1}^N g_{j,s} \cos \frac{2\pi ks}{N}$,

$$b_{j,k}^{(2)}(y) = \frac{2}{N} \sum_{s=1}^N g_{j,s} \sin \frac{2\pi ks}{N},$$

$$c_{m,k}^{(1)} = \frac{2}{N} \sum_{s=1}^N T_{m,s} \cos \frac{2\pi ks}{N},$$

$$c_{m,k}^{(2)} = \frac{2}{N} \sum_{s=1}^N T_{m,s} \sin \frac{2\pi ks}{N}.$$

For the coefficients $a_{j,k}^{(1)}(y)$, $a_{j,k}^{(2)}(y)$ the solution is in the form (7) (FDSES). If $\lambda_k = \mu_k$, we have the FDS.

7. The Solution of the Problem in Two Layers

For 2 layers (M=2) we consider the following parameters: $N = 10, y_0 = 0, y_1 = 1, y_2 = 3, k_1 = 10, k_2 = 1, T_2(x) = 0, f_1(x, y) = 0, \gamma_1 = \gamma_2 = 0, \alpha_1 = \alpha_2 = 1, f_2(x, y) = P\delta(y - 2) \sin(2\pi x)$ or $f_2(x, y) = P \sin(2\pi x), T_1(x) = \sin(\pi x)$ - for the BCs of the first kind, $T_1(x) = \sin(2\pi x)$ - for the periodic BCs, where $P = 10, \delta(y - 2)$ - is the Dirac delta function. In this case the analytical solution depends only on two eigenvectors X_1, X_2 and w^1, w_*^1 . Numerical results in the y direction are obtained in uniform grid with 6 and 30 grid points.

7.1. The Exact Solution

The exact solution for the BCs of first kind, using two eigenvectors $X_1, X_2, (\sin(\pi x) = \sqrt{l/2}X_1(x), \sin(2\pi x) = \sqrt{l/2}X_2(x))$, is in the following form:

$$\begin{cases} u_1(x, y) = a_{1,1}(y) \sin(\pi x) + a_{1,2}(y) \sin(2\pi x), \\ u_2(x, y) = a_{2,1}(y) \sin(\pi x) + (a_{2,2}(y) - P \frac{p_1(y)}{2\pi k_2}) \sin(2\pi x), \end{cases} \tag{16}$$

where

$$\begin{cases} a_{1,1}(y) = C_{1,1} \sinh(\pi y) + B_{1,1} \cosh(\pi y), \\ a_{1,2}(y) = C_{1,2} \sinh(2\pi y) + B_{1,2} \cosh(2\pi y), \\ a_{2,1}(y) = C_{2,1} \sinh(\pi(y - 1)) + B_{2,1} \cosh(\pi(y - 1)), \\ a_{2,2}(y) = C_{2,1} \sinh(2\pi(y - 1)) + B_{2,1} \cosh(2\pi(y - 1)), \end{cases} \tag{17}$$

$$B_{1,1} = 1, \quad C_{1,1} = -\frac{\cosh(\pi) + \kappa_1 \sinh(\pi) \tanh(2\pi)}{\sinh(\pi) + \kappa_1 \cosh(\pi) \tanh(2\pi)}, \quad \kappa_1 = \frac{k_1}{k_2},$$

$$B_{2,1} = C_{1,1} \sinh(\pi) + B_{1,1} \cosh(\pi), \quad C_{2,1} = \kappa_1(C_{1,1} \cosh(\pi) + B_{1,1} \sinh(\pi)),$$

$$B_{1,2} = 0, \quad C_{1,2} = \frac{Pp_1(3)}{2\pi k_2(\sinh(2\pi) + \kappa_1 \cosh(2\pi) \sinh(4\pi))},$$

$$C_{2,2} = \kappa_1 C_{1,2} \cosh(2\pi), \quad B_{2,2} = C_{1,2} \sinh(2\pi),$$

$$p_1(y) = [0, y \in [1, 2]; \sinh(2\pi(y - 2)), \quad y \in [2, 3]]$$

for $f_2(x, y) = P\delta(y-2) \sin(2\pi x) p_1(y) = (\cosh(2\pi(y-1))-1)/(2\pi)$ for $f_2(x, y) = P \sin(2\pi x)$.

For the periodic BCs, using eigenvectors $X_1, X_1^*, (\sin(2\pi x) = \frac{\sqrt{l}}{2i}(X_1(x) - X_1^*(x)), X_1^*(x) = X_{-1}(x))$, the solution is in the form:

$$u_1(x, y) = a_{1,1}(y) \sin(2\pi x), \quad u_2(x, y) = a_{2,1}(y) \sin(2\pi x), \tag{18}$$

where

$$\begin{cases} a_{1,1}(y) = C_{1,1} \sinh(2\pi y) + B_{1,1} \cosh(2\pi y) \\ a_{2,1}(y) = C_{2,1} \sinh(2\pi(y - 1)) + B_{2,1} \cosh(2\pi(y - 1)) - \frac{Pp_1(y)}{2\pi k_2}, \end{cases} \quad (19)$$

$$B_{1,1} = 1,$$

$$C_{1,1} = -B_{1,1} \frac{\cosh(2\pi) + \kappa_1 \sinh(2\pi) \tanh(4\pi) - Pp_1(3)/(2\pi k_2 \cosh(4\pi))}{\sinh(2\pi) + \kappa_1 \cosh(2\pi) \tanh(4\pi)},$$

$$B_{2,1} = C_{1,1} \sinh(2\pi) + B_{1,1} \cosh(2\pi), C_{2,1} = \kappa_1(C_{1,1} \cosh(2\pi) + B_{1,1} \sinh(2\pi)).$$

7.2. The Averaging Solution

For the averaging solution $F_1 = 0, F_2 = P \sin(2\pi x)$ for

$$f_2 = P \sin(2\pi x), \quad F_2 = 0.5P \sin(2\pi x),$$

$$f_2 = P\delta(y - 2) \sin(2\pi x)$$

we have two linear algebraic equations (10):

$$\begin{cases} (B_1 + 1)e_1 + B_1 e_2 = a_1(U_2 - U_1) - b_1(U_1 - T_1) \\ A_2 e_1 + (A_2 + 1)e_2 = a_2(T_2 - U_2) - b_2(U_2 - U_1), \end{cases} \quad (20)$$

where $B_1 = \frac{G_2}{G_1 + G_2} A_2 = \frac{G_1}{G_1 + G_2}, a_1 = \frac{3}{G_1 + G_2}, b_1 = \frac{3}{G_1}, b_2 = \frac{3}{G_1 + G_2}, a_2 = \frac{3}{G_2}.$

The solution of (20) is in the form:

$$\begin{cases} e_1 = c_{1,1}U_1(x) + c_{1,2}U_2(x) + c_{1,0}T_1(x) \\ e_2 = c_{2,1}U_1(x) + c_{2,2}U_2(x) + c_{2,0}T_1(x), \end{cases} \quad (21)$$

where

$$c_{1,1} = -\frac{b_{0,3} + b_1(A_2 + 1)}{b_{0,1}}, \quad c_{1,2} = \frac{b_{0,3} + B_1 a_2}{b_{0,1}}, \quad c_{1,0} = \frac{b_1(A_2 + 1)}{b_{0,1}},$$

$$c_{2,1} = \frac{b_{0,2} + b_1 A_2}{b_{0,1}}, \quad c_{2,2} = -\frac{b_{0,2} + (B_1 + 1)a_2}{b_{0,1}}, \quad c_{2,0} = -\frac{b_1 A_2}{b_{0,1}},$$

$$b_{0,1} = (B_1 + 1)(A_2 + 1), \quad b_{0,2} = A_2 a_1 + (B_1 + 1)b_2, \quad b_{0,3} = (A_2 + 1)a_1 + B_1 b_2.$$

The solution of the 2 ODEs (9) for the *BCs of the first kind* can be obtained using two orthonormal eigenvectors $X_1(x), X_2(x)$ in the following form:

$$U_1(x) = a_1^1 \sin(\pi x) + a_2^1 \sin(2\pi x), U_2(x) = a_1^2 \sin(\pi x) + a_2^2 \sin(2\pi x),$$

where the coefficients a_j^k satisfy the following system of algebraic equations:

$$\begin{cases} -k_1\lambda_1 a_1^1 + 2(c_{1,1}a_1^1 + c_{1,2}a_1^2 + c_{1,0}) = 0 \\ -k_2\lambda_1 a_1^2 + (c_{2,1}a_1^1 + c_{2,2}a_1^2 + c_{2,0}) = 0 \\ -k_1\lambda_2 a_2^1 + 2(c_{1,1}a_2^1 + c_{1,2}a_2^2) = 0 \\ -k_2\lambda_2 a_2^2 + (c_{2,1}a_2^1 + c_{2,2}a_2^2) + \beta P = 0. \end{cases} \tag{22}$$

where $\beta = 1$ for $f_2 = P \sin(2\pi x)$, $\beta = 0.5$ for $f_2 = P\delta(y - 2) \sin(2\pi x)$.

The solution for *the periodic BCs* can be obtained using the biorthonormal eigenvectors $X_1(x), X_1^*(x)$ similarly to (18) in following form:

$$U_1(x) = a_1^1 \sin(2\pi x), \quad U_2(x) = a_1^2 \sin(2\pi x),$$

where the coefficients a_1^1, a_1^2 can be determined from the following system of 2 algebraic equations:

$$\begin{cases} -k_1\lambda_1 a_1^1 + 2(c_{1,1}a_1^1 + c_{1,2}a_1^2 + c_{1,0}) = 0 \\ -k_2\lambda_1 a_1^2 + c_{2,1}a_1^1 + c_{2,2}a_1^2 + c_{2,0} + \beta P = 0. \end{cases} \tag{23}$$

We have the following solution of (22,23):

$$\begin{aligned} a_1^1 &= (2c_{1,2}(c_{2,0} + p_2P) - 2c_{1,0}(c_{2,2} - k_2\lambda_1))/det_1, \\ a_1^2 &= (2c_{2,1}c_{1,0} - (c_{2,0} + \beta p_2P)(2c_{1,1} - k_1\lambda_1))/det_1, \\ det_1 &= (2c_{1,1} - k_1\lambda_1)(c_{2,2} - k_2\lambda_1) - 2c_{1,2}c_{2,1}, \\ a_2^1 &= 2c_{1,2}P/det_2, a_2^2 = -\beta P(2c_{1,1} - k_1\lambda_2)/det_2, \\ det_2 &= (2c_{1,1} - k_1\lambda_2)(c_{2,2} - k_2\lambda_2) - 2c_{1,2}c_{2,1}, \end{aligned}$$

where $p_2 = 1$ for the periodic BCs, $p_2 = 0$ for the BCs of the first kind.

Since

$$\begin{cases} m_1(x) = \frac{1}{3k_1(G_1+G_2)}(6(U_2(x) - U_1(x)) - e_1(x)(G_1 + 3G_2) - 2e_2(x)G_2) \\ m_2(x) = \frac{1}{3k_2(G_1+G_2)}(6(U_2(x) - U_1(x)) + e_2(x)(G_2 + 3G_1) + 2e_1(x)G_1), \end{cases} \tag{24}$$

the functions $u_1(x, y), u_2(x, y)$ can be determined from (8).

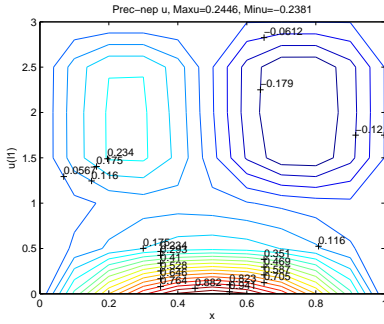


Figure 1: Exact solution

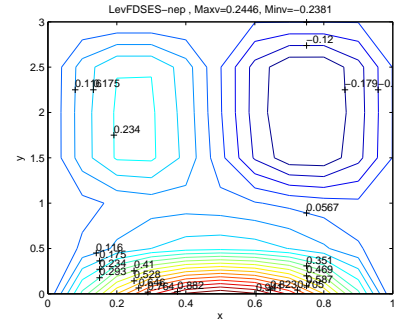


Figure 2: FDSES solution

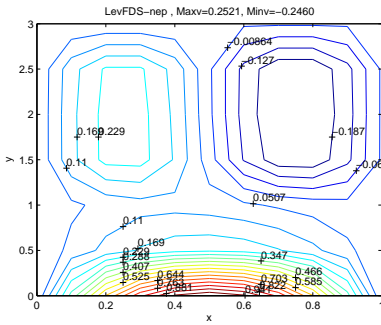


Figure 3: FDS solution

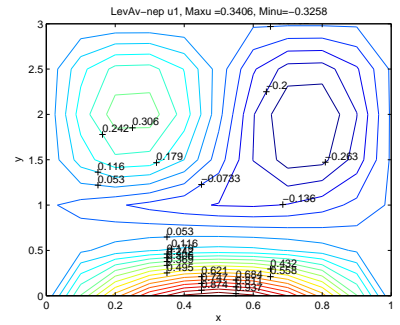


Figure 4: Averaging solution

7.3. The Solutions of the FDS and FDSES

The analytical *FDS solution* of (13 - 15) can be obtained in the following form:

$$\begin{cases} \bar{v}_{1,1}(y) = C_{1,1} \sinh(\sqrt{d_1}y) + B_{1,1} \cosh(\sqrt{d_1}y), & y \in [0, 1], \\ \bar{v}_{1,2}(y) = C_{1,2} \sinh(\sqrt{d_2}y) + B_{1,2} \cosh(\sqrt{d_2}y), & y \in [0, 1], \\ \bar{v}_{2,1}(y) = C_{2,1} \sinh(\sqrt{d_1}(y - 1)) + B_{2,1} \cosh(\sqrt{d_1}(y - 1)), & y \in [1, 3], \\ \bar{v}_{2,2}(y) = C_{2,2} \sinh(\sqrt{d_2}(y - 1)) + B_{2,2} \cosh(\sqrt{d_2}(y - 1)), & y \in [1, 3], \end{cases} \quad (25)$$

where the coefficients $C_{j,k}, B_{j,k}$ can be obtained from (17), similarly the coefficients $a_{j,k}$ can be determined, where the values $\pi, 2\pi$ are replaced with $\sqrt{d_1}, \sqrt{d_2}$, and $B_{1,1} = \sqrt{N/2}$. For the FDS $d_1 = \mu_1, d_2 = \mu_2$, but for the FDSES $d_1 = \lambda_1, d_1 = \lambda_2$.

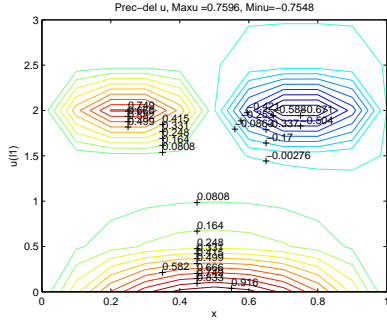


Figure 5: Exact solution for the δ -function

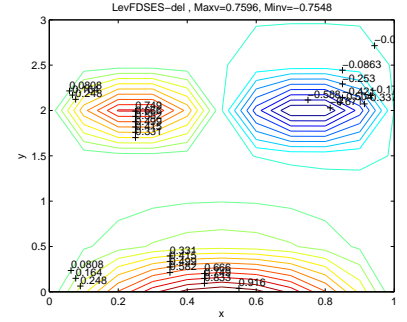


Figure 6: FDSES solution for the δ -function

For the *periodic BCs*, using the eigenvectors w^1, w^1_* , ($\sin(2\pi x_j) = \frac{\sqrt{N}}{2i}(w^1(x_j) - w^1_*(x_j))$, $w^1_*(x_j) = w^{N-1}(x_j)$, $\mu_{N-1} = \mu_1$), we have the following results:

$$\begin{cases} \bar{v}_{1,1}(y) = C_{1,1} \sinh(\sqrt{d_1}y) + B_{1,1} \cosh(\sqrt{d_1}y), & y \in [0, 1], \\ \bar{v}_{2,1}(y) = C_{2,1} \sinh(\sqrt{d_1}(y-1)) + B_{2,1} \cosh(\sqrt{d_1}(y-1)) - \\ -P \frac{p_1(3)}{k_2 \sqrt{d_1}}, & y \in [1, 3], \end{cases} \quad (26)$$

where the coefficients $C_{j,k}, B_{j,k}$ can be obtained from (19). Similarly, the coefficients $a_{j,k}$, where the value 2π is replaced with $\sqrt{d_1}$. For the FDS $d_1 = \mu_1$, but for the FDSES $d_1 = \lambda_1$ (we have the exact solution[7]).

8. Some Numerical Results

For the *BCs of the first kind* the numerical results can be represented in the following way:

1) $f_2(x, y) = 10 \sin(2\pi)$ - the exact solution (see Figure 1), the FDSES solution (see Figure 2), the FDS solution (see Figure 3), the averaging solution (see Figure 4),

2) $f_2(x, y) = 10 \sin(2\pi)\delta(y-2)$ - the exact solution (see Figure 5), the FDSES solution (see Figure 6), the FDS solution (see Figure 7), the averaging solution (see Figure 8).

We have the following results for the maximal and minimal values Mu and mu of the $u_2(x, y)$ solution (for the exact and the FDSES solutions

$$Mu = 0.2446, \quad mu = -0.2381, \quad f_2(x, y) = 10 \sin(2\pi); \quad Mu = 0.7596,$$

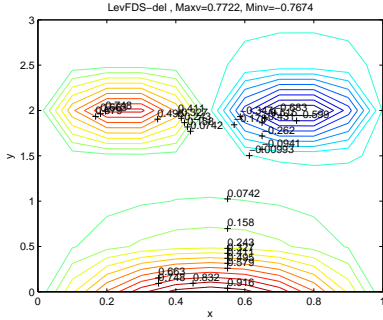


Figure 7: FDS solution for the δ - function

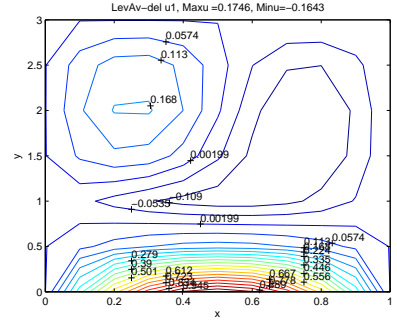


Figure 8: Averaging solution for the δ - function

$$\mu = -0.7548, \quad f_2(x, y) = 10 \sin(2\pi)\delta(y - 2) :$$

- 1) for the FDS and $f_2(x, y) = 10 \sin(2\pi)$, $Mu = 0.2521$, $mu = -0.2460$,
- 2) for the FDS and $f_2(x, y) = 10 \sin(2\pi)\delta(y - 2)$, $Mu = 0.7722$, $mu = -0.7674$.

For the periodic BCs we have the following results:

- 1) $f_2(x, y) = 10 \sin(2\pi)$ - the exact and the FDSES solutions (see Figure 10), the FDS solution (see Figure 11), the averaging solution (see Figure 12),
- 2) $f_2(x, y) = 10 \sin(2\pi)\delta(y - 2)$ - the exact and the FDSES solutions (see Figure 9), the FDS solution (see Figure 13), the averaging solution (see Figure 14).

Using the different p order ($p = 2; 4; 6; 8$) finite difference approximations, we have following results for the maximal and minimal values of the solution $u_2(x, y)$ (for the exact and the FDSES solutions- $mu = \pm 0.2401$, $f_2(x, y) = 10 \sin(2\pi)$; $mu = \pm 0.7568$, $f_2(x, y) = 10 \sin(2\pi)\delta(y - 2)$) :

- 1) For $f_2(x, y) = 10 \sin(2\pi)$, $mu = \pm 0.2480(p = 2)$; $\pm 0.2405(p = 4)$; $\pm 0.2401(p = 6)$; $\pm 0.2401(p = 8)$,
- 2) For $f_2(x, y) = 10 \sin(2\pi)\delta(y - 2)$, $mu = \pm 0.7694(p = 2)$; $\pm 0.7575(p = 4)$; $\pm 0.7569(p = 6)$; $\pm 0.7568(p = 8)$.

We can see, that the FDSES method is exact. It also follows from the theorems in [7]. The maximum relative error value for the averaging method is approximately 10%.

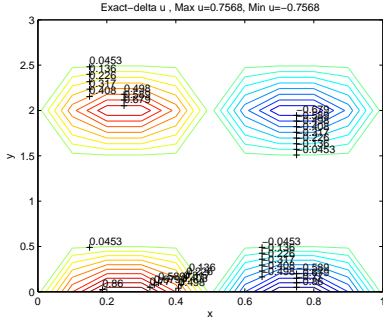


Figure 9: FDSES solution for the δ -function

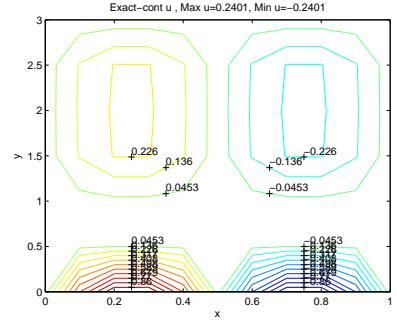


Figure 10: FDSES solution

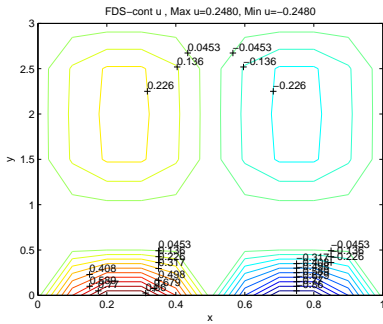


Figure 11: FDS solution

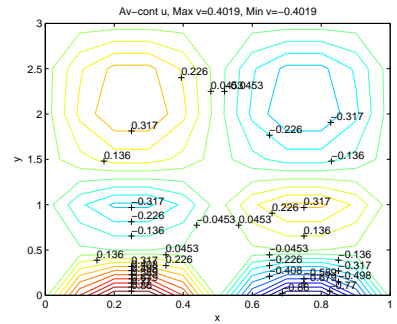


Figure 12: Averaged solution

9. Conclusion

The 2-D diffusion problem in the M layered domain is described by the boundary-value-problem for the PDEs system with piece-wise constant diffusion coefficients. By the system approximation we obtain the 1-D boundary-value-problem for the system of M ODEs. This algorithm can be used, for example, for solving problems of a metal concentration in layered peat blocks.

For this problem the FDSES method provides the most precise results. In some cases the FDSES method is exact.

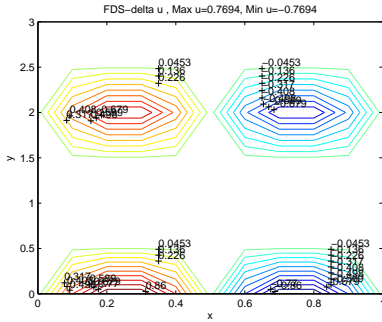


Figure 13: FDS solution with δ - function

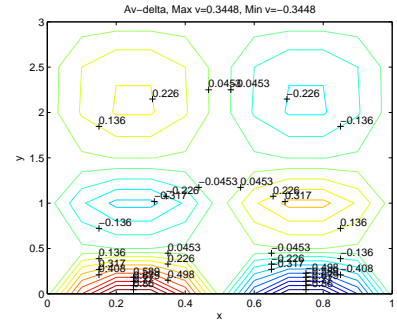


Figure 14: Averaged solution with δ - function

Acknowledgements

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