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SIMPLE METHODS OF ENGINEERING CALCULATION FOR SOLVING MULTI-SUBSTANCES TRANSFER PROBLEM IN MULTI-LAYER MEDIA

H.KALIS and I.KANGRO

Institute of Mathematics Latvian Academy of Sciences and University of Latvia

Akadēmijas laukums 1, LV-1524 Rīga, Latvia

E-mail: kalis@lanet.lv

Rēzekne Higher Education Institution, Departament of engineering science

Atbrīivoŝanas aleja 90, LV-4601, Rēzekne, Latvija

E-mail: kangro@cs.ru.lv

Abstract. In this paper we study the simple algorithms for modelling the transfer problem of different m substances ($m \geq 2$, an example is concentration, moisture, heat, e.c.) in multi-layer domain. The approximation of corresponding initial boundary value problem of the system of m partial differential equations (PDEs) is based on the finite volume method. This procedure allows one to reduce the 2D transfer problem described by a system of PDEs to initial value problem for a system of ordinary differential equations (ODEs) of the first or second order. The corresponding scalar transfer problems are considered in [4, 5]. In a stationary case the exact finite difference vector scheme is obtained. An example of the problem in two layer media is considered.
Key words: System of PDEs, vector finite difference schemes

1. The Mathematical Model

The plate with thickness l is a multilayer media Ω of N layers $\Omega = \{x : x \in \Omega_k, k = \overline{1,N}\}$, where each layer is given in the form

$$\Omega_k = \{x : x_{k-1} \leq x \leq x_k\},\ x_0 = 0, x_N = l,$$

$x_k (k = \overline{1, N-1})$ are interfaces of the layers (the interior grid points in the finite difference methods). We shall consider the initial - boundary value problem for finding vector-functions $u_k = u_k(x,t) = (u_k^{(1)}(x,t), \ldots, u_k^{(m)}(x,t))^T$ from the following system of PDEs in every layer $\Omega_k, k = \overline{1,N}$:

$$G_k \frac{\partial u_k}{\partial t} = \frac{\partial}{\partial x}\Big(L_k \frac{\partial u_k}{\partial x}\Big) - Q_k, \quad x \in \Omega, t > 0, \tag{1.1}$$

where G_k is a quadratic matrix $m \times m$ with constant elements $\gamma_k^{(i,j)}$ such that $\det(G_k) \neq 0$, L_k is a quadratic positive definite matrix $m \times m$ with constant elements $l_k^{(i,j)}$, Q_k is vector-column $m \times 1$ with constant elements $q_k^{(j)}, i, j = \overline{1, m}$.

The system of PDEs (1.1) can be rewritten in the following form:

$$\frac{\partial}{\partial x}\Big(L_k \frac{\partial u_k(x,t)}{\partial x}\Big) = F_k, \quad k = \overline{1, N}, \tag{1.2}$$

where $F_k = G_k \dot{u}_k(x,t) + Q_k,\ \dot{u}_k = \dfrac{\partial u_k}{\partial t}$. We have the following continuity conditions on the interior surfaces $x = x_k, k = \overline{1, N-1}$:

$$\begin{cases} u_k(x_k,t) = u_{k+1}(x_k,t) \\ L_k u_k'(x_k,t) = L_{k+1} u_{k+1}'(x_k,t), \end{cases} \tag{1.3}$$

and boundary conditions on the exterior surfaces $x = x_0 = 0,\ x = x_N = l$:

$$\begin{cases} L_1 u_1'(0,t) = \alpha_0(u_1(0,t) - T_0) \\ L_N u_N'(l,t) = \alpha_l(T_l - u_N(l,t)), \end{cases} \tag{1.4}$$

where $u' = \dfrac{\partial u}{\partial x},\ \alpha_0, \alpha_l$ are diagonal-matrixes with constant elements

$$\alpha_0^{(j)},\ \alpha_l^{(j)}, \quad j = \overline{1, m},$$

T_0, T_l are known vector-functions with elements $T_0^{(j)}(t), T_l^{(j)}(t), j = \overline{1, m}$.

For the initial condition at $t = 0$ we define

$$u_k(x,0) = \phi(x), k = \overline{1, N}, \tag{1.5}$$

where ϕ is known vector-column. If the elements of matrix α_0 or α_l are equal to infinity ($\alpha_0 = \infty$, or $\alpha_l = \infty$,) then we have the first kind boundary conditions

$$u_1(0,t) = T_0,\ u_N(l,t) = T_l. \tag{1.6}$$

2. The 2-Layer Problem and Approximation of Integrals

Using the method of finite volumes for scalar functions (see [3]) we obtain the following exact vector finite-difference scheme with respect to grid points $x_k,\ k = \overline{0, N}$ and given function F_k [5]:

$$L_1 h_1^{-1}(u_1 - u_0) - \alpha_0(u_0 - T_0) = \bar{R}_0^+, \tag{2.1}$$

$$L_{k+1}h_{k+1}^{-1}(u_{k+1}-u_k) - L_k h_k^{-1}(u_k - u_{k-1}) = \bar{R}_k,\ k=\overline{1, N-1}, \tag{2.2}$$

$$\alpha_l(T_l - u_N) - L_N h_N^{-1}(u_N - u_{N-1}) = \bar{R}_N^-. \tag{2.3}$$

The right side of expressions $R_k^{\pm}$ contain integrals of derivatives $u_k(x,t)$. In the stationary case $\dot{u}_k = 0$ this scheme is exact. For non-stationary problem $\dot{u}_k \neq 0$, to approximate the integrals we considered different quadrature formulas [5].

Now we restrict to the case of only two layers, that is

$$N=2,\ \ x_1 = h_1,\ \ x_2 = l = h_1 + h_2,\ \ \alpha_0 = \infty,\ \ u_0 = T_0.$$

Then the unknown vector-functions are u_1, u_2. In the non-stationary case the finite-difference scheme is given by

$$\begin{cases} L_2 h_2^{-1}(u_2 - u_1) - L_1 h_1^{-1}(u_1 - T_0) = G_2 R_1^+ + G_1 R_1^- + I_1 \\ \alpha_l(T_l - u_2) - L_2 h_2^{-1}(u_2 - u_1) = G_2 R_2^{-1} + I_2^-, \end{cases} \tag{2.4}$$

where $I_1 = I_1^- + I_1^+$, and

$$R_1^- = \frac{1}{h_1}\int_0^{h_1} x\dot{u}_1(x,t)\,dx = h_1 J_3,\ \ R_1^+ = \frac{1}{h_2}\int_{h_1}^{l}(l-x)\dot{u}_2(x,t)\,dx = h_2 J_1,$$

$$R_2^- = \frac{1}{h_2}\int_{h_1}^{l}(x-h_1)\dot{u}_2(x,t)\,dx = h_2 J_2, \quad J_1 = \int_0^1 (1-\bar{x})V_2(\bar{x})\,d\bar{x},$$

$$J_2 = \int_0^1 \bar{x}V_2(\bar{x})\,d\bar{x},\ \ \bar{x} = \frac{x-h_1}{h_2}, \quad V_2(\bar{x}) = \dot{u}_2(h_1 + h_2\bar{x}, t),$$

$$J_3 = \int_0^1 \bar{x}V_1(\bar{x})\,d\bar{x},\ \ \bar{x} = \frac{x}{h_1}, \quad V_1(\bar{x}) = \dot{u}_1(h_1\bar{x}, t).$$

In the non-stationary case we compute integrals $J_j,\ j=1,2,3$ approximately with quadrature formulas in the following way ($j=1,2$):

$$J_j = A_1^{(j)}V_2(0) + A_2^{(j)}V_2(1) + A_3^{(j)}V_2'(1) + B_1^{(j)}V_2''(0) + B_2^{(j)}V_2''(1) + r_j, \tag{2.5}$$

$$J_3 = A_1^{(3)}V_1(0) + A_2^{(3)}V_1(1) + B_1^{(3)}V_1''(0) + B_2^{(3)}V_1''(1) + r_3, \tag{2.6}$$

where for $j=1,2$:

$$r_j = \frac{h_2^5}{5!}\frac{\partial^5 \dot{u}_2(\xi_j,t)}{\partial x^5}C_j,\ \xi_j \in (h_1, l),\ \ r_3 = \frac{h_1^4}{4!}\frac{\partial^4 \dot{u}_1(\xi_3,t)}{\partial x^4}C_3,\ \xi_3 \in (0, h_1)$$

are the vector-errors terms, $A_k^{(j)}, B_k^{(j)}, C_j (j,k=1,2,3)$ are the indefinite coefficients.

Using the power functions $\bar{x}^i, i=0,1,...$ in (2.5)–(2.6) similarly the scalar case [3] for the fixed coordinates of vectors $V_1(\bar{x}), V_2(\bar{x})$ we get the following two systems of linear algebraic equations for $A_k^{(j)}, B_k^{(j)}$:

$$\begin{cases} \dfrac{1}{(i+1)(i+2)} = A_1^{(1)}0^i + A_2^{(1)} + iA_3^{(1)} + i(i-1)(B_1^{(1)}0^{i-2} + B_2^{(1)}), \\ \dfrac{1}{i+2} = A_1^{(2)}0^i + A_2^{(2)} + iA_3^{(2)} + i(i-1)(B_1^{(2)}0^{i-2} + B_2^{(2)}), \quad i = \overline{0,4}, \end{cases} \tag{2.7}$$

and

$$\frac{1}{i+2} = A_1^{(3)}0^i + A_2^{(3)} + i(i-1)(B_1^{(3)}0^{i-2} + B_2^{(3)}), \quad i = \overline{0,3}, \tag{2.8}$$

where $0^i = 1$ for $i \leq 0$.

Simple computations show that the solutions of the corresponding systems (2.7) – (2.8) are given by

$$A_1^{(1)} = \frac{7}{30}, \ A_2^{(1)} = \frac{4}{15}, \ A_3^{(1)} = -\frac{1}{10}, \ B_1^{(1)} = -\frac{1}{180}, \ B_2^{(1)} = \frac{1}{72},$$

$$A_1^{(2)} = \frac{1}{15}, \ A_2^{(2)} = \frac{13}{30}, \ A_3^{(2)} = -\frac{1}{10}, \ B_1^{(2)} = -\frac{1}{360}, \ B_2^{(2)} = \frac{1}{90},$$

$$A_1^{(3)} = \frac{1}{6}, \ A_2^{(3)} = \frac{1}{3}, \ B_1^{(3)} = -\frac{7}{360}, \ B_2^{(3)} = -\frac{1}{45}.$$

Constants C_j in the residual r_j are determined using power functions $\bar{x}^4$ and $\bar{x}^5$:

$$C_1 = -\frac{13}{630}, \quad C_2 = -\frac{4}{315}, \quad C_3 = \frac{1}{10}.$$

Using the vector difference equations (2.4) and the right-side integrals approximations (2.5), (2.6) with neglected error terms $r_j, j = \overline{1,3}$ we have the following vector system of linear ODEs of second order ($\dot{u}_0 = \ddot{u}_0 = 0$, $\ddot{u} = \dfrac{\partial^2 u}{\partial t^2}$, $\alpha_0 = \infty$) :

$$\begin{cases} G_2h_2[A_1^{(1)}\dot{u}_1 + (A_2^{(1)} - h_2A_3^{(1)}L_2^{-1})\dot{u}_2 + h_2^2B_1^{(1)}L_2^{-1}G_2\ddot{u}_1 \\ +h_2^2B_2^{(1)}L_2^{-1}G_2\ddot{u}_2] + G_1h_1[A_2^{(3)}\dot{u}_1 + h_1^2B_2^{(3)}L_1^{-1}G_1\ddot{u}_1] \\ \qquad +I_1 = h_2^{-1}L_2(u_2 - u_1) - h_1^{-1}L_1(u_1 - T_0), \end{cases} \tag{2.9}$$

$$\begin{cases} G_2h_2[A_1^{(2)}\dot{u}_1 + (A_2^{(2)} - h_2A_3^{(2)}L_2^{-1})\dot{u}_2 + h_2^2B_1^{(2)}L_2^{-1}G_2\ddot{u}_1 \\ +h_2^2B_2^{(2)}L_2^{-1}G_2\ddot{u}_2] + I_2^- = \alpha_l(T_l - u_2) - h_2^{-1}L_2(u_2 - u_1). \end{cases} \tag{2.10}$$

The initial conditions for ODEs (2.9), (2.10) are given by

$$\begin{cases} u_1(0) = \phi(h_1), \ \ u_2(0) = \phi(l), \ \ \dot{u}_1(0) = G_1^{-1}(L_1\phi''(h_1) - Q_1), \\ \dot{u}_2(0) = G_2^{-1}(L_2\phi''(l) - Q_2). \end{cases} \tag{2.11}$$

Here one should take in account that from (1.1)–(1.6) it follows:

$$V_2'(1) = h_2 \frac{\partial}{\partial x}\dot{u}_2(l,t) = -h_2 L_2^{-1}\alpha_l \dot{u}_2,$$

$$V_1''(0) = h_1^2 \frac{\partial^2}{\partial x^2}\dot{u}_1(0,t) = h_1^2 \frac{\partial}{\partial t} u_1''(0,t) = h_1^2 L_1^{-1} G_1 \ddot{u}_0,$$

$$V_1''(1) = h_1^2 \frac{\partial^2}{\partial x^2}\dot{u}_1(h_1,t) = h_1^2 L_1^{-1} G_1 \ddot{u}_1,$$

$$V_2''(0) = h_2^2 L_2^{-1} G_2 \ddot{u}_1, \quad V_2''(1) = h_2^2 L_2^{-1} G_2 \ddot{u}_2.$$

Remark 1. If $\alpha_0 = \alpha_l = \infty, u_0 = T_0, u_2 = T_l$, then the vector finite–difference equation follows from (2.4):

$$h_2^{-1} L_2(T_l - u_1) - h_1^{-1} L_1(u_1 - T_0) = G_2 h_2 J_1 + G_1 h_1 J_3 + I_1, \qquad (2.12)$$

where

$$J_1 = A_1^{(1)} V_2(0) + A_2^{(1)} V_2(1) + B_1^{(1)} V_2''(0) + B_2^{(1)} V_2''(1) + r_1,$$

$$r_1 = \frac{h_2^4}{4!}\frac{\partial^4 \dot{u}_2(\xi_1,t)}{\partial x^4} C_1, \quad \xi_1 \in (h_1, l),$$

$$A_1^{(1)} = \frac{1}{3}, \quad A_2^{(1)} = \frac{1}{6}, \quad B_1^{(1)} = -\frac{1}{45}, \quad B_2^{(1)} = -\frac{7}{360}, \quad C_1 = \frac{1}{10}.$$

Therefore the system of ODEs of second order ($\dot{u}_0 = \dot{u}_2 = 0$, $\ddot{u}_0 = \ddot{u}_2 = 0$) is given in the following form

$$\begin{cases} G_2 h_2 [A_1^{(1)} \dot{u}_1 + h_2^2 B_1^{(1)} L_2^{-1} G_2 \ddot{u}_1] + G_1 h_1 [A_2^{(3)} \dot{u}_1 \\ + h_1^2 B_2^{(3)} L_1^{-1} G_1 \ddot{u}_1] + I_1 = h_2^{-1} L_2 (T_l - u_1) - h_1^{-1} L_1 (u_1 - T_0). \end{cases} \qquad (2.13)$$

If integrals J_1, J_3 are approximated without the derivatives then we get the following system of ODEs of first order

$$\frac{1}{3}(h_2 G_2 + h_1 G_1)\dot{u}_1 + I_1 = h_2^{-1} L_2 (T_l - u_1) - h_1^{-1} L_1 (u_1 - T_0). \qquad (2.14)$$

3. Some Numerical Results and Examples

Example 1. Let assume that

$$m = 2, \;\; Q_1 = Q_2 = 0, \;\; L_1 = L_2 = L, \;\; T_0 = T_l = 0, \;\; G_1 = G_2 = G, \;\; l = 1,$$

$$\phi(x) = (\sin(\pi x), \sin(\pi x)_T, \quad h_1 = h_2 = h = 0.5,$$

$$L = E = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}, \;\; G = \begin{pmatrix} 1 & 0 \\ 1 & 1 \end{pmatrix}, \;\; G^2 = \begin{pmatrix} 1 & 0 \\ 2 & 1 \end{pmatrix}, \;\; G^{-1} = \begin{pmatrix} 1 & 0 \\ -1 & 1 \end{pmatrix},$$

then the exact solution of PDEs problem (1.1)–(1.6) is given by

$$u(x,t) = (\exp(-\pi^2 t)\sin(\pi x), \exp(-\pi^2 t)(1+\pi^2 t)\sin(\pi x))^T,$$

$$u_1 = u(h,t) = (\exp(-\pi^2 t), \exp(-\pi^2 t)(1+\pi t))^T.$$

This is the solution of ODEs

$$G\ddot{u}_1 = \pi u_1.$$

From the first order ODEs (2.14) we get the vector initial-value problem

$$G\dot{u}_1 = -12u_1, \quad u_1(0) = (1,1)^T,$$

and the solutions with error $O(h^2)$ is given by

$$u_1 = u(h,t) = \big(\exp(-12t), \exp(-12t)(1+12t)\big)^T.$$

Therefore the value π^2 is replaced with 12.

From second order ODEs (2.13) we get the following initial-value problem

$$\begin{cases} b_1 G^2 \ddot{u}_1 + a_1 G\dot{u}_1 + u_1 = 0 \\ u_1(0) = (1,1)^T, \;\; \dot{u}_1(0) = -G^{-1}(\pi^2,\pi^2)^T = (-\pi^2, 0)^T, \end{cases} \tag{3.1}$$

where

$$b_1 = 0.5h^4(B_1^{(1)} + B_2^{(3)}) = \frac{89}{11520}, \;\; a_1 = 0.5h^2(A_1^{(1)} + A_3^{(3)}) = \frac{7}{48}.$$

Let denote $u_1^{(1)} = y, u_1^{(2)} = z$, then we have the initial-value problem for system of two ODEs of the second order

$$\begin{cases} b_1\ddot{y} + a_1\dot{y} + y = 0, \; y(0) = 1, \; \dot{y}(0) = -\pi^2, \\ b_1\ddot{z} + a_1\dot{z} + z = -2b_1\ddot{y} - a_1\dot{y}, \; z(0) = 1, \; \dot{z}(0) = 0. \end{cases} \tag{3.2}$$

The solution with error $O(h^4)$ is given by

$$y(t) = D_1\exp(\mu_1 t) + D_2\exp(\mu_2 t),$$
$$z(t) = D_1(1-\mu_1 t)\exp(\mu_1 t) + D_2(1-\mu_2 t)\exp(\mu_2 t),$$

where $\mu_{1,2} = -a_1/(2b_1) \pm \sqrt{(a_1/(2b_1))^2 - 1/b_1}$,

$$D_1 = \frac{\mu_2 + \pi^2}{\mu_2 - \mu_1}, \quad D_2 = \frac{-\pi^2 + \mu_1}{\mu_2 - \mu_1}.$$

The results of calculations obtained by MAPLE are presented in Table 1, where u_*, v_* are exact values of $u_1^{(1)}, u_1^{(2)}$, $u_{p2}, v_{p2}-$ values with approximation $O(h^2)$ and u_{p4}, v_{p4} values with approximation $O(h^4)$.

Table 1. The values of vector $u(0.5,t)$ at different time moments t.

t	u_*	v_*	u_{p4}	v_{p4}	u_{p2}	v_{p2}
.1	.3727	.7406	.383	.750	.301	.663
.2	.1389	.4131	.147	.428	.091	.308
.3	.0518	.2051	.056	.218	.027	.126
.4	.0193	.0955	.021	.104	.008	.048
.5	.0072	.0427	.008	.048	.002	.017

Example 2. In [2] the model textile package is described by the system of two equations for transfer of heat and moisture given in the following form

$$\begin{cases} a_1 \dfrac{\partial C}{\partial t} - b_1 \dfrac{\partial T}{\partial t} = c_1 \dfrac{\partial^2 C}{\partial x^2} \\ -b_2 \dfrac{\partial C}{\partial t} + a_2 \dfrac{\partial T}{\partial t} = c_2 \dfrac{\partial^2 T}{\partial x^2}, \end{cases} \tag{3.3}$$

where $a_i, b_i, c_i (i = 1, 2)$, are positive constants. The system of two PDEs (3.3) is written in form (1.1), where $Q = 0, u = (C, T)^T$ is the vector-column,

$$G = \begin{pmatrix} a_1 & -b_1 \\ -b_2 & a_2 \end{pmatrix}, \quad L = \begin{pmatrix} c_1 & 0 \\ 0 & c_2 \end{pmatrix}, \quad \det(G) > 0.$$

Example 3. In [1] for modelling heat (temperature T) and moisture (M) transport in wood plate or paper sheet the following system of PDEs is considered

$$\begin{cases} \dfrac{\partial T}{\partial t} = \dfrac{\partial}{\partial x}(D_h \dfrac{\partial M}{\partial x} + E_h \dfrac{\partial T}{\partial x}) \\ \dfrac{\partial M}{\partial t} = \dfrac{\partial}{\partial x}(D_m \dfrac{\partial M}{\partial x} + E_m \dfrac{\partial T}{\partial x}), \end{cases} \tag{3.4}$$

where D_h, D_m are the heat and moisture coefficients of the moisture gradients, E_h, E_m are the corresponding coefficients of the temperature gradients. The system (3.4) for constant coefficients is given in the matrix form (1.1), where $Q = 0$, $G = E$,

$$L = \begin{pmatrix} D_h & E_h \\ D_m & E_m \end{pmatrix}, \quad u = (T, M)^T, \quad D_h > 0, \quad D_h E_m - E_h D_m > 0.$$

4. Conclusions

The 2D transfer problem described by an initial boundary value problem of the system of PDEs with piece-wise constant coefficients is approximated by the initial value problem of a system of ODEs of the first or second order. For increasing the accuracy of approximation, the second order differential equations are taken instead of initial value problem of system of first order ODEs (a corresponding example in two layer domain is consider). Such a procedure allows us to obtain a simple engineering algorithm for solving mass transfer equations for different substances in multilayered domain.

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