ON THE NUMERICAL MODELING OF POLLUTION IN AIR, WATER AND SOIL

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Abstract: *Model pollution in air, water and soil are generally described by a system of PDEs on unbounded domain. Transformation of the independent variable is used to convert the problem for nonlinear air pollutionon to finite computational domain. Then we construct a fitted finite volume difference scheme. Some results from computations are presented.*

Key words: *Nonlinear air, water and soil pollution, Chemical reaction, Infinite domain, Log-transformation, Degeneracy, Non-negativity preservation, Finite volume method.*

INTRODUCTION

Environmental problems are becoming more and more important for our world and their importance will even increase in the future. High pollution of air, water and soil may cause damage of plants, animals and humans.

An air (or water, or soil) pollution model is generally described by a system of PDE-s for calculating the concentrations of a number of chemical species (pollutants and components of the air, water and soil that interact with the pollutant) in a large 3-D domain (part of the atmosphere above the studied geographical region, rivers, channels etc.) [4], [6], [7]

$$\frac{\partial c_s}{\partial t} = -\frac{\partial (uc_s)}{\partial x} - \frac{\partial (vc_s)}{\partial y} - \frac{\partial (wc_s)}{\partial z} + \frac{\partial}{\partial x}\left(K_s^x \frac{\partial c_s}{\partial x}\right) + \frac{\partial}{\partial y}\left(K_s^y \frac{\partial c_s}{\partial y}\right) + \frac{\partial}{\partial z}\left(K_s^z \frac{\partial c_s}{\partial z}\right) + F_s$$
$$+R_s(c_1, c_2, \ldots, c_S) - (k_{1,s} + k_{2,s})c_s, \quad s = 1, 2, \ldots, S,$$

where c_s are the *concentrations* of the chemical species; u, v and w are wind velocities, K_s^x, K_s^y and K_s^z are the diffusion components; F_s are the emissions; $k_{1,s}$, $k_{2,s}$ are dry/wet deposition coefficients and $R_s(c_1, c_2, \ldots, c_S)$ are non-linear functions describing the chemical reactions between the species under consideration [4], [6], [7]. Typical is the case $R_s(c_1, c_2, \ldots, c_S) = \sum_{i=1}^{S} \gamma_{s,i} c_i + \sum_{i=1, j=1}^{S} \beta_{s,i,j} c_i c_j, \ s = 1, 2, \ldots, S,$ where $\gamma_{s,i}$ and $\beta_{s,i,j}$ are constants.

For such complex models operator splitting is very often applied in order to achieve sufficient accuracy as well as efficiency of the numerical solution. Although the splitting is a crucial step in efficient numerical treatment of the model, after discretization of the large computational domain each sub-problem becomes itself a huge computational task. Here we will concentrate on a non-stationary sub-model of a horizontal advection-diffusion with chemistry, emissions and deposition, see [4], [5], [7]:

$$\frac{\partial c_s}{\partial t} - \frac{\partial}{\partial z}\left(K_s(z) \frac{\partial c_s}{\partial z}\right) + w \frac{\partial c_s}{\partial z} - R_s(c_1, c_2, \ldots, c_S) = Q_s(t)\delta\left(z - z_s^*\right), \quad z \in (0, \infty), \quad t \in (0, T], \qquad (1)$$

$$\frac{\partial c_s}{\partial z}(t, 0) = \delta_s c_s(t, 0), \quad \delta_s = const \geq 0, \qquad \lim_{z \to \infty} c_s(t, z) = 0, \quad t \in [0, T], \qquad (2)$$

$$c_s(0, z) = c_{s,0}, \quad z \in [0, \infty), \quad s = 1, 2, \ldots, S. \qquad (3)$$

The rest of the paper is organized as follows. In Section 2 we introduce the transformed differential problem and derive the fitted finite volume discretization. In Section 3 we present some results from computational experiments. At the end we formulate some conclusions.

THE TRANSFORMED PROBLEM AND NUMERICAL METHOD

In the numerical scheme it is not convenient to corporate the boundary condition at infinity. For the simplest case of (1) (one linear advection-diffusion equation) discrete transparent boundary conditions are constructed and analyzed in [3] while in [2] the transformation

$$z = \frac{1}{2a}\ln\left(\frac{1+\xi}{1-\xi}\right), \quad \xi \in \Omega = (0,1) \Leftrightarrow \xi = \frac{e^{2az}-1}{e^{2az}+1}, \quad z \in (0,\infty)\,, \tag{4}$$

is used. Here a is a stretching factor. Using transformation [4], the system (1) and the respective boundary and initial conditions (2)–(3) in the computational domain become

$$\frac{\partial C_s}{\partial t} - a^2\left(1-\xi^2\right)^2 k_s(\xi)\frac{\partial^2 C_s}{\partial \xi^2} + a\left(1-\xi^2\right)\left(2a\xi k_s(\xi) + w - a\left(1-\xi^2\right)\frac{\partial k_s(\xi)}{\partial \xi}\right)\frac{\partial C_s}{\partial \xi}$$
$$-r_s(C_1, C_2, \ldots, C_S) = Q_s(t)\delta\left(\xi - \xi_s^*\right), \quad \xi \in (0,1), \quad t \in (0,T], \tag{5}$$

$$a\frac{\partial C_s}{\partial \xi}(t,0) = \delta_s C_s(t,0), \qquad C_s(t,1) = 0, \quad t \in [0,T], \tag{6}$$

$$C_s(0,z) = C_{s,0}, \quad \xi \in [0,1], \quad s = 1,2,\ldots,S\,. \tag{7}$$

We have used the notations $r_s(C_1, C_2, \ldots, C_S) \equiv R_s(c_1(t,z(\xi)), c_2(t,z(\xi)), \ldots, c_S(t,z(\xi)))$, $C_s(t,\xi) \equiv c_s(t,z(\xi)),\; k_s(\xi) = K_s(z(\xi))$.

We rewrite the system (5) in divergent form:

$$\frac{\partial C_s}{\partial t} = \frac{\partial}{\partial \xi}\left(p_s(\xi)\frac{\partial C_s}{\partial \xi} + q_s(\xi)C_s\right) + B_s(\xi, C_1, C_2, \ldots, C_S) + f_s(t,\xi), \quad (t,\xi) \in (0,T]\times(0,1), \tag{8}$$

$$p_s(\xi) = a^2(1-\xi^2)^2 k_s(\xi),\; q_s(\xi) = a(1-\xi^2)\left[2a\xi k_s(\xi) - w\right],\; B_s(\xi, C_1, \ldots, C_S) = r_s(C_1, \ldots, C_S) - d_s(\xi)C_s,$$

$$d_s(\xi) = 2a^2(1-3\xi^2)k_s(\xi) + 2a^2\xi\left(1-\xi^2\right)\frac{\partial k_s(\xi)}{\partial \xi} + 2aw\xi\,,$$

where $f_s(t,\xi)$ is a regularization of the Dirac delta-function, $s = 1,2,\ldots,S$.

Considering the process of pollutant transport and diffusion in the atmosphere (and in the water and the soil) the concentrations $C_1, C_2, \ldots, C_S$ of pollutants can not be negative if they are non-negative in the initial state $t = 0$ for all $\xi \in (0,1)$. This property is called *non-negativity preservation* and it is well studied for single heat-diffusion equation.

Let the interval $[0,1]$ be subdivided into N intervals $I_i = [\xi_i, \xi_{i+1}],\; i = 1,2,\ldots,N$ with $0 = \xi_1 < \xi_2 < \ldots < \xi_{N+1} = 1$ and $h_i = \xi_{i+1} - \xi_i$. We set $\xi_{i-1/2} = 0.5\left(\xi_{i-1} + \xi_i\right)$, $\xi_{i+1/2} = 0.5\left(\xi_i + \xi_{i+1}\right)$, $\hbar_i = \xi_{i+1/2} - \xi_{i-1/2}$ for $i = 2,3,\ldots,N$.

A. *Internal nodes.* We integrate equation (8) on the cell $[\xi_{i-1/2}, \xi_{i+1/2}]$ and applying the mid-point quadrature rule to all the integrals with exception to the second one we obtain

$$\left.\frac{\partial C_s}{\partial t}\right|_{(t,\xi_i)} \hbar_i = \left.\left(p_s(\xi)\frac{\partial C_s}{\partial \xi} + q_s(\xi)C_s\right)\right|_{(t,\xi_{i+1/2})} - \left.\left(p_s(\xi)\frac{\partial C_s}{\partial \xi} + q_s(\xi)C_s\right)\right|_{(t,\xi_{i-1/2})}$$
$$+\hbar_i\left[B_s\left(\xi, C_1, \ldots, C_S\right) + f_s(t,\xi)\right]\Big|_{(t,\xi_i)}\,. \tag{9}$$

Further at the derivation of the discrete equations we follow the methodology in [1], [2]. Let us rewrite equation (9) in the form

$$\frac{\partial C_{s,i}}{\partial t}\hbar_i = (1-\xi_{i+1/2}^2)\rho_{s,i+1/2} - (1-\xi_{i-1/2}^2)\rho_{s,i-1/2} + \hbar_i\left(B_{s,i} + f_{s,i}\right), \tag{10}$$

$$\rho_s \equiv \rho_s\left(C_s\right) = a^2(1-\xi^2)k_s(\xi)\frac{\partial C_s}{\partial \xi} + \left(2a^2\xi k_s(\xi) - aw\right)C_s . \tag{11}$$

We need to derive an approximation of the continuous flux ρ_s in the point $\xi_{i+1/2}$, $i = 2,3,\ldots,N-1$. To do this, we consider the *two-point* BVP

$$\left(l_{s,i+1/2}(1-\xi^2)V_s' + M_{s,i+1/2}V_s\right)' = 0, \quad \xi \in I_i , \qquad V_s(\xi_i) = C_{s,i}, \qquad V_s(\xi_{i+1}) = C_{s,i+1} \tag{12}$$

where $l_s(\xi) = a^2 k_s(\xi)$, $m_s(\xi) = 2a^2\xi k_s(\xi) - aw$, $l_{s,i+1/2} = c_s(\xi_{i+1/2})$, $m_{s,i+1/2} = b_s(\xi_{i+1/2})$. Integrating equation from (12) yields the first-order linear equation. Solving this equation and using the boundary conditions gives

$$\rho_{s,i+1/2} = m_{s,i+1/2}\frac{\Delta_{s,i}(\xi_{i+1})C_{s,i+1} - \Delta_{s,i}(\xi_i)C_{s,i}}{\Delta_{s,i}(\xi_{i+1}) - \Delta_{s,i}(\xi_i)}, \quad \alpha_{s,i} = \frac{m_{s,i+1/2}}{l_{s,i+1/2}}, \quad \Delta_{s,i}(\xi_i) = \left(\frac{1+\xi_i}{1-\xi_i}\right)^{\frac{\alpha_{s,i}}{2}} . \tag{13}$$

In a similar way we approximate $\rho_{s,i-1/2}$ for $i = 2,3,\ldots,N$. For approximation of $\rho_{s,N+1/2}$ we solve the BVP

$$\left(\overline{l}_{s,N+1/2}(1-\xi)V_s' + m_{s,N+1/2}V_s\right)' = M_2, \quad V_s(\xi_N) = C_{s,N}, \quad V_s(\xi_{N+1}) = 0,$$

where $\overline{l}_s(\xi) = a^2(1+\xi)k_s(\xi)$. After some calculation for the flux $\rho_{s,N+1/2}$ we get

$$\rho_{s,N+1/2} = 0.5\left[C_{s,N+1}\left(\overline{l}_{s,N+1/2} + m_{s,N+1/2}\right) - C_{s,N}\left(\overline{l}_{s,N+1/2} - m_{s,N+1/2}\right)\right].$$

B. *Boundary nodes*. To approximate the boundary condition on the left vertical boundary $\xi = 0$ we proceed as for the internal grid nodes, but integrating equation (8) on the interval (i. e. in the semi-interval by ξ) to get

$$\frac{\partial C_{s,1}}{\partial t}\frac{h_1}{2} = (1-\xi_{3/2}^2)\rho_{s,3/2} - (1-\xi_1^2)\rho_{s,1} + \frac{h_1}{2}\left(B_{s,1} + f_{s,1}\right).$$

From (13) for $i = 1$ we get the approximation for $\rho_{s,3/2}$. For $(1-\xi_1^2)\rho_{s,1}$, where $\xi_1 = 0$, using the expression for ρ_s (11) and the boundary condition (6) we find $(1-\xi_1^2)\rho_{s,1} = a\left(\delta_s k_s(0) - w\right)C_{s,1}$. On the right vertical boundary $\xi_1 = 1$ we have $C_{s,N+1} = 0$.

Finally, for the space approximation we obtain the ODE non-linear system of equations for $C_{s,i}(t)$, $s = 1,2,\ldots,S$, $i = 1,2,\ldots,N+1$:

$$\frac{\partial C_{s,1}}{\partial t}\frac{h_1}{2} = -e_{s,1,1}C_{s,1} + e_{s,1,2}C_{s,2} + \frac{h_1}{2}\left[B_s(\xi_1, C_{1,1}, C_{2,1},\ldots,C_{S,1}) + f_{s,1}(t)\right],$$

$$\frac{\partial C_{s,i}}{\partial t}\hbar_i = e_{s,i,i-1}C_{s,i-1} - e_{s,i,i}C_{s,i} + e_{s,i,i+1}C_{s,i+1} + \hbar_i\left[B_s(\xi_i, C_{1,i}, C_{2,i},\ldots,C_{S,i}) + f_{s,i}(t)\right], \quad i = 2,3,\ldots,N,$$

$$C_{s,N+1} = 0,$$

$$e_{s,1,1} = \frac{(1-\xi_{3/2}^2)m_{s,3/2}\Delta_{s,1}(\xi_1)}{\Delta_{s,1}(\xi_2) - \Delta_{s,1}(\xi_1)} + a\left(\delta_s k_s(\xi_1) - w\right), \quad e_{s,i,i-1} = \frac{(1-\xi_{i-1/2}^2)m_{s,i-1/2}\Delta_{s,i-1}(\xi_{i-1})}{\Delta_{s,i-1}(\xi_i) - \Delta_{s,i-1}(\xi_{i-1})}, \; i = 2,3,\ldots,N,$$

$$e_{s,i,i} = \frac{(1-\xi_{i+1/2}^2)m_{s,i+1/2}\Delta_{s,i}(\xi_i)}{\Delta_{s,i}(\xi_{i+1}) - \Delta_{s,i}(\xi_i)} + \frac{(1-\xi_{i-1/2}^2)m_{s,i-1/2}\Delta_{s,i-1}(\xi_i)}{\Delta_{s,i-1}(\xi_i) - \Delta_{s,i-1}(\xi_{i-1})}, \quad i = 2,3,\ldots,N-1;$$

$$e_{s,i,i+1} = \frac{(1-\xi_{i+1/2}^2)m_{s,i+1/2}\Delta_{s,i}(\xi_{i+1})}{\Delta_{s,i}(\xi_{i+1}) - \Delta_{s,i}(\xi_i)}, \; i = 1,2,\ldots,N-1, \quad e_{s,N,N+1} = 0.5(1-\xi_{N+1/2}^2)\left(\overline{l}_{s,N+1/2} + m_{s,N+1/2}\right),$$

$$e_{s,N,N} = 0.5(1-\xi_{N+1/2}^2)\left(\overline{l}_{s,N+1/2} - m_{s,N+1/2}\right) + \frac{(1-\xi_{N-1/2}^2)m_{s,N-1/2}\Delta_{s,N-1}(\xi_N)}{\Delta_{s,N-1}(\xi_N) - \Delta_{s,N-1}(\xi_{N-1})} .$$

In order to discretize the problem with respect to t we introduce the mesh $0 = t_1 < t_2 < \ldots < t_{M+1} = T$, $\Delta t_j = t_{j+1} - t_j$. Then, the fully implicit scheme can be written in the form

$$\frac{C_{s,1}^{j+1} - C_{s,1}^{j}}{\Delta t_j}\frac{h_1}{2} = -e_{s,1,1}C_{s,1}^{j+1} + e_{s,1,2}C_{s,2}^{j+1} + \frac{h_1}{2}\left[B_s(\xi_1, C_{1,1}^{j+1}, C_{2,1}^{j+1}, \ldots, C_{S,1}^{j+1}) + f_{s,1}^{j+1}\right], \tag{14}$$

$$\frac{C_{s,i}^{j+1} - C_{s,i}^{j}}{\Delta t_j}\hbar_i = e_{s,i,i-1}C_{s,i-1}^{j+1} - e_{s,i,i}C_{s,i}^{j+1} + e_{s,i,i+1}C_{s,i+1}^{j+1} + \hbar_i\left[B_s(\xi_i, C_{1,i}^{j+1}, \ldots, C_{S,i}^{j+1}) + f_{s,i}^{j+1}\right], i = 2,3,\ldots,N, \tag{15}$$

$$C_{s,N+1}^{j+1} = 0,\ s = 1,2,\ldots,S, \tag{16}$$

where $C_{s,i}^{j} = C_s(t_j, \xi_i)$. To solve the non-linear system (14)–(16) we have used Newton's method, which leads to a linear system of equations.

RESULTS AND DISCUSSION

The components of the system are the nitric oxide (NO), nitrogen dioxide (NO_2) and ozone (O_3), denoted by u_1, u_2 and u_3 respectively. We assume that the nitrogen dioxide is released at source locations and concentrations of nitric oxide are measured. A simplified model of chemical reactions in the system is

$NO \to O_3 \xrightarrow{k_1} NO_2$, $\quad NO_2 \xrightarrow{k_2} NO + O_3$, with rates $k_1 = 1000$, $k_2 = 2000$.

To show the efficiency and usefulness of the discretization method, various test problems with different choices of parameters were solved. In the numerical experiment we approximate the Dirac-delta function by the function

$$\delta_h(\xi) = \frac{2h - |\xi - \xi^*|}{4h^2},\quad \xi \in \left[\xi^* - 2h, \xi^* + 2h\right] \text{ and } 0, \xi \notin \left[\xi^* - 2h, \xi^* + 2h\right].$$

For the numerical results presented here, we have used the following functions and values of the coefficients in the problem under consideration: $S = 3, K_1(z) = 1$, $K_2(z) = K_3(z) = 5$, $w = 1$, $Q_1(t)$, $Q_2(t) = 1 - t$, $Q_3(t) = 0$, $z_1^* = 20$, $z_2^* = 85$, $\delta_1 = \delta_2 = \delta_3 = 0$, $T = 1$, $c_{1,0} = c_{2,0} = 0$, $c_{3,0} = 2$, $a = 0.005$, $R_s = \gamma_{s,2}c_2 + \beta_{s,1,3}c_1c_3$, $s = 1,2,3$, where $\gamma_{1,2} = -\gamma_{2,2} = \gamma_{3,2} = 2000$, $\beta_{1,1,3} = -\beta_{2,1,3} = \beta_{3,1,3} = -1000$. A part of these data are taken from [5]. Fig. 1, 2 and 3 show the numerical computed concentrations $c_1(t,z)$, $c_2(t,z)$ and $c_3(t,z)$.

We have used the Runge method for practical estimation of the rate of convergence of the scheme *with respect to the space variable* at fixed value of $t = T = 1$. We have used three inserted grids with 100, 200 and 400 subintervals respectively by ξ and $\Delta t = \Delta t_j = 0.001$. A part of the results from the calculations for the rate of convergence are presented in the Table.

CONCLUSIONS AND FUTURE WORK

In this work we have considered a one-dimensional nonlinear problem of pollution in air, water and soil. We have used a log-transformation that makes the original problem, defined on a semi-infinite interval, to another one on the interval $(0,1)$. We have derived a fitted volume difference scheme that preserves the non-negativity property of the differential problem solution as numerical experiments show. Detail experimental and theoretical analysis will be very interesting.

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ξ	0.00	0.01	0.02	0.03	0.04	0.05	0.06	0.07	0.08	0.09	0.10	0.11	0.12	0.13
n_1	11.04	9.27	7.63	6.16	4.89	3.84	3.04	2.49	2.26	3.08	0.08	1.40	2.12	2.27
n_2	11.04	9.28	7.63	6.16	4.89	3.84	3.04	2.46	2.07	1.40	1.25	0.54	1.57	2.13
n_3	1.74	1.07	2.17	-1.67	5.15	3.84	3.04	2.46	2.07	1.40	1.25	0.54	1.57	2.13
ξ	0.26	0.27	0.28	0.29	0.30	0.35	0.36	0.37	0.38	0.39	0.40	0.41	0.42	0.43
n_1	23.97	19.62	17.23	14.96	12.79	4.00	2.90	2.15	1.89	1.99	1.67	1.19	1.59	1.69
n_2	23.98	19.63	17.24	14.97	12.80	4.01	2.93	2.24	1.97	2.03	1.79	1.40	1.68	1.79
n_3	2.01	2.00	1.94	0.44	5.25	2.57	2.06	1.79	1.82	1.48	2.79	2.17	-1.96	1.64

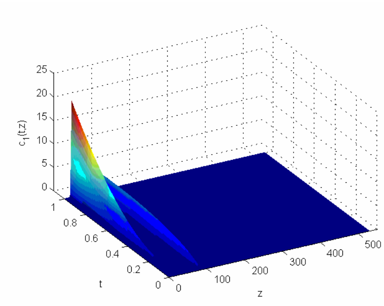

Fig. 1. $c_1(t,z)$.

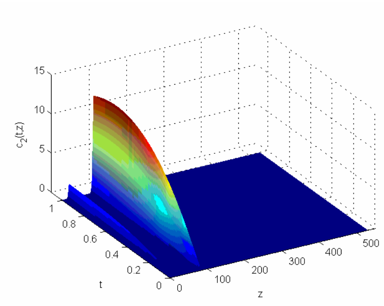

Fig. 2. $c_2(t,z)$.

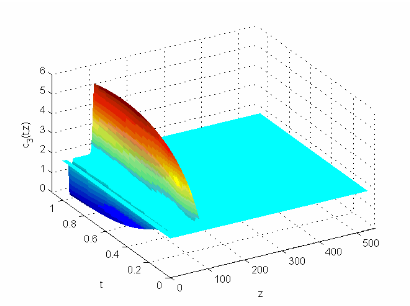

Fig. 3. $c_3(t,z)$.

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