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ON NUMERICAL MODELLING FOR DISPERSION OF ACTIVE POLLUTANTS FROM A ELEVATED POINT SOURCE[1]

DANG QUANG A * and NGUYEN DONG ANH **

Abstract. *This paper deals with a problem of dispersion of active pollutants from a elevated point source in the atmosphere. The problem is firstly reduced to some relatively independent three-dimensional problems, which are of type solved by us in earlier works. In this work we investigate further properties of the numerical solution, namely, the dependence of the solution on the coefficient of reflection and absorption of the bedding surface and the coefficient of transformation. A comparison of numerical solutions of problems with various boundary conditions is given. The conclusions derived from the theory are completely agreed with the physical picture of the problem.*

1. SETTING OF THE PROBLEM

Suppose that at the point $(0, 0, H)$ of the half-space $\{(x, y, z), z \geq 0\}$ there is located a source of emission of gaseous or particulate pollutants, for example, the stack of a thermoelectric station or a chemical plant. These pollutants disperse in the atmosphere and can be converted from one form to another. This conversion may be described by the following chain

$$\varphi_1 \to \varphi_2 \to \varphi_3 \to \cdots \tag{1.1}$$

where φ_i is the concentration of the i-th pollutant.

We assume that the chain (1.1) includes more than N components ($N \geq 2$) and that the components $N+1, N+2, \ldots$ are not essential and may be neglected. Therefore, we shall consider (1.1) with N first components.

According to Marchuk [1] the transport-diffusion process of active pollutants is governed by the following equations

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$$
\begin{aligned}
&\overline{A}\varphi_1 + \sigma_1\varphi_1 = f \\
&\overline{A}\varphi_2 + \sigma_2\varphi_2 = \tilde{\sigma}_1\varphi_1 \\
&\cdots\cdots\cdots \\
&\overline{A}\varphi_N + \sigma_N\varphi_N = \tilde{\sigma}_{N-1}\varphi_{N-1}\,,
\end{aligned}
\tag{1.2}
$$

where

$$\overline{A} = \frac{\partial}{\partial t} + \operatorname{div}(\mathbf{u}.) - w_g\frac{\partial}{\partial z} - \mu\frac{\partial^2}{\partial x^2} - \mu\frac{\partial^2}{\partial y^2} - \frac{\partial}{\partial z}\nu\frac{\partial}{\partial z}\,, \tag{1.3}$$

$\mathbf{u} = (u, v, w)$ is wind velocity, ν and μ are the vertical and horizontal diffusion coefficients, respectively, σ_i, $\tilde{\sigma}_i$ $(i = \overline{1, N})$ are the rate coefficients of conversion of the i-th pollutant in general and to $i+1$-th pollutant, respectively, $w_g = \text{constant} > 0$,

$$f = Q\,\delta(x)\,\delta(y)\,\delta(z-H)\,, \tag{1.4}$$

the constant Q is the power of the emission source, and δ is Dirac delta function.

We pose the following boundary conditions on φ_i $(i = \overline{1, N})$

$$\varphi_i = 0\,, \quad x, y \to \pm\infty\,, \quad z \to +\infty\,, \tag{1.5}$$

$$\frac{\partial\varphi_i}{\partial z} = \alpha\varphi_i\,, \quad z = 0\,.$$

Since the source of the emission has constant power, we may regard the process described above as a stationary process for each short interval of time during which the wind velocity slightly changes. Hence, instead of (1.2) we treat the system

$$
\begin{aligned}
&A\varphi_1 + \sigma_1\varphi_1 = f\,, \\
&A\varphi_2 + \sigma_2\varphi_2 = \tilde{\sigma}_1\varphi_1\,, \\
&\cdots\cdots\cdots \\
&A\varphi_N + \sigma_N\varphi_N = \tilde{\sigma}_{N-1}\varphi_{N-1}\,,
\end{aligned}
\tag{1.6}
$$

where

$$A = \operatorname{div}(\mathbf{u}.) - w_g\frac{\partial}{\partial z} - \mu\frac{\partial^2}{\partial x^2} - \mu\frac{\partial^2}{\partial y^2} - \frac{\partial}{\partial z}\nu\frac{\partial}{\partial z} \tag{1.7}$$

The numbers $\sigma_1, \ldots, \sigma_N$ are assumed to be distinct and positive except for σ_N, which may be zero if the N-th pollutant is not converted to another forms. In practice this assumption is usually satisfied.

The problem of dispersion of active aerosols was studied by some authors. For example, Marchuk [1] obtained the solution for the (x, y)-model with constant wind velocity, Pal and Sinha [2] constructed numerical solution for the (x, z)-model with $N = 2$ in the layer $z \leq \mathcal{H}$.

In this paper we shall consider the system (1.6) together with the boundary condition (1.5) in the half-space $z \geq 0$.

2. REDUCTION OF THE PROBLEM TO N INDEPENDENT PROBLEMS

In principle we can solve (1.5) - (1.6) by sequential finding φ_1 and φ_i $(i = \overline{2, N})$ after φ_{i-1} is known. But we observe that the right-hand side of the equation for φ_1 has the special form (1.4), while the one of the equation for φ_i $(i = \overline{2, N})$ contains the just computed function φ_{i-1}. Besides, each problem for φ_i is posed in the half-space $z \geq 0$, i.e. in a three-dimensional domain. Therefore, solving it both analytically and numerically is very difficult and combersome. Moreover, the problems for φ_i $(i \geq 2)$ should be solved in sequence one after another. Hence, the total computation time required should be too long.

In order to overcome the above difficulties we suggest first to reduce the problem (1.5) - (1.6) to N independent problems with right-hand side of the same form as (1.4). In their turn, the independent problems may be led to problems in two-dimensional domain and may be solved concurrently on individual processors of a parallel computing system.

Below we present a way to reduce (1.5) - (1.6) to N independent problems.

For $i = \overline{2, N}$ we multiply the first equation of (1.6) by a_{i1}, the second equation by a_{i2} and so on, the i-th equation by a_{ii}, where $a_{i1}, a_{i2}, \ldots, a_{ii}$ are undetermined coefficients. After summing up from 1 to i just multiplied equations we obtain

$$\begin{aligned} &A(a_{i1}\varphi_1 + \cdots + a_{ii}\varphi_i) + (a_{i1}\sigma_1 - a_{i2}\tilde{\sigma}_1)\varphi_1 + \\ &+ (a_{i2}\sigma_2 - a_{i3}\tilde{\sigma}_2)\varphi_2 + \cdots + a_{ii}\sigma_i\varphi_i = a_{i1} f \quad (i = \overline{2, N}) \end{aligned} \tag{2.1}$$

We can choose a_{ij} $(j = \overline{1, i})$ so that

$$(a_{i1}\sigma_1 - a_{i2}\tilde{\sigma}_1)\varphi_1 + \cdots + (a_{i,i-1}\sigma_{i-1} - a_{ii}\tilde{\sigma}_{i-1})\varphi_{i-1} + \\ + a_{ii}\sigma_i\varphi_i = \sigma_i(a_{i1}\varphi_1 + \cdots + a_{ii}\varphi_i), \tag{2.2}$$

e.g.

$$a_{ij} = \frac{\tilde{\sigma}_i}{\sigma_j - \sigma_i} a_{i,j+1}, \quad j = i-1, \dots, 1, \\ a_{ii} \neq 0 \text{ is arbitrary}, \quad i = \overline{2, N}. \tag{2.3}$$

Now putting

$$\Phi_1 = \varphi_1, \quad \Phi_i = a_{i1}\varphi_1 + \cdots + a_{ii}\varphi_i, \quad i = \overline{2, N}, \tag{2.4}$$

$$F_1 = f, \quad F_i = a_{i1} f, \quad i = \overline{2, N}, \tag{2.5}$$

we get the equations

$$A\Phi_i + \sigma_i \Phi_i = F_i, \quad i = \overline{1, N} \tag{2.6}$$

and boundary conditions

$$\Phi_i = 0, \quad |x|, |y|, z \to \infty, \\ \frac{\partial \Phi_i}{\partial z} = \alpha \Phi_i, \quad z = 0, \quad i = \overline{1, N}. \tag{2.7}$$

Thus, we have reduced the problem (1.5) - (1.6) to N independent problem (2.6), (2.7) for $i = \overline{1, N}$ with the special right-hand side (2.5). After solving these problems we can calculate φ_i $(i = \overline{1, N})$ from (2.4).

Theorem 2.1. *Let Φ_i $(i = \overline{1, N})$ be the solution of Problem (2.6) - (2.7). Then φ_i $(i = \overline{1, N})$ calculated from (2.4) are the solution of Problem (1.5) - (1.6).*

Proof. First, we introduce the following notations

$$\mathcal{A} = \begin{pmatrix} 1 & 0 & 0 & \cdots & 0 \\ a_{21} & a_{22} & 0 & \cdots & 0 \\ a_{31} & a_{32} & a_{33} & \cdots & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ a_{N1} & a_{N2} & a_{N3} & \cdots & a_{NN} \end{pmatrix},$$

$$\mathcal{L} = \begin{pmatrix} A+\sigma_1 & 0 & 0 & \cdots & 0 & 0 \\ -\tilde{\sigma}_1 & A+\sigma_2 & 0 & \cdots & 0 & 0 \\ 0 & -\tilde{\sigma}_2 & A+\sigma_3 & \cdots & 0 & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & 0 & \cdots & -\tilde{\sigma}_{N-1} & A+\sigma_N \end{pmatrix},$$

$$\mathcal{D} = \begin{pmatrix} A+\sigma_1 & 0 & \cdots & 0 \\ 0 & A+\sigma_2 & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & A+\sigma_N \end{pmatrix},$$

$$\varphi = \begin{pmatrix} \varphi_1 \\ \varphi_2 \\ \vdots \\ \varphi_N \end{pmatrix}, \quad \Phi = \begin{pmatrix} \Phi_1 \\ \Phi_2 \\ \vdots \\ \Phi_N \end{pmatrix}, \quad G = \begin{pmatrix} f \\ 0 \\ \vdots \\ 0 \end{pmatrix}, \quad F = \begin{pmatrix} f \\ a_{21}f \\ \vdots \\ a_{N1}f \end{pmatrix}.$$

Then Systems (1.6), (2.6) and Relation (2.4) may be written respectively in the forms

$$\mathcal{L}\varphi = G, \tag{2.8}$$

$$\mathcal{D}\varphi = F, \tag{2.9}$$

and

$$\mathcal{A}\varphi = \Phi. \tag{2.10}$$

From the last relation we derive

$$\varphi = \mathcal{A}^{-1}\Phi. \tag{2.11}$$

Since φ also satisfies the same boundary conditions as Φ does, the theorem will be proved if we show that φ defined by (2.11) satisfies (2.8).

For this purpose we note that the elements a_{ij} of $\mathcal{A}$ given by (2.3) satisfy the matrix equation $\mathcal{A}\mathcal{L} = \mathcal{D}\mathcal{A}$ or

$$\mathcal{A}\mathcal{L}\mathcal{A}^{-1} = \mathcal{D}. \tag{2.12}$$

Indeed, setting $a_{ij} = 0$ for $j > i$ we have

$$(\mathcal{A}\mathcal{L})_{ij} = a_{ij}(A+\sigma_j) - a_{i,j+1}\tilde{\sigma}_j,$$
$$(\mathcal{D}\mathcal{A})_{ij} = (A+\sigma_i)a_{ij}, \quad i = \overline{1,N}, \; j \le i.$$

Equating corresponding elements of the matrices we obtain (2.3).

Now we can rewrite (2.9) in the form

$$\mathcal{A}\mathcal{L}\mathcal{A}^{-1}\Phi = F\,.$$

In view of (2.11) we have $\mathcal{A}\mathcal{L}\varphi = F$. Whence, taking into account the obvious fact that $\mathcal{A}G = F$ we get (2.8). Thus, the proof is complete.

3. NUMERICAL INVESTIGATION OF THE INDEPENDENT PROBLEMS

As seen above Problem (1.5) - (1.6) is reduced to N independent problems of the form

$$u\frac{\partial\varphi}{\partial x} + v\frac{\partial\varphi}{\partial y} + (w - w_g)\frac{\partial\varphi}{\partial z} - \mu\frac{\partial^2\varphi}{\partial x^2} - \mu\frac{\partial^2\varphi}{\partial y^2} - \frac{\partial}{\partial z}\nu\frac{\partial\varphi}{\partial z} +$$
$$+\sigma\varphi = Q\delta(x)\delta(y)\delta(z-H)\,, \tag{3.1}$$
$$\varphi = 0\,, \quad |x|,\, |y|,\, z \to \infty\,,$$
$$\frac{\partial\varphi}{\partial z} = \alpha\varphi\,, \quad z = 0\,.$$

Also, this problem under the assumptions that

$$u = u(z) > 0,\ v = w = 0,\ \mu = k_0 u,\ k_0 = \text{constant} > 0 \tag{3.2}$$

is reduced to the following problem (see [3,4])

$$u\frac{\partial\varphi}{\partial x} - w_g\frac{\partial\varphi}{\partial z} - \frac{\partial}{\partial z}\nu\frac{\partial\varphi}{\partial z} + \sigma\varphi = 0\,,\ x > 0\,, \tag{3.3}$$

$$u\varphi = Q\delta(z-H)\,, \quad x = 0$$
$$\varphi = 0\,, \quad z \to \infty\,, \tag{3.3a}$$
$$\frac{\partial\varphi}{\partial z} = \alpha\varphi\,, \quad z = 0\,.$$

A numerical method for solving this problem was proposed and investigated in [4,5]. In this section we study dependence of numerical solution of the problem on σ, α and compare the solutions of problems with other boundary conditions.

First we recall some facts from [4, 5].

On the grid

$$\overline{\Omega} = \{z_i = ih_z, x_j = jh_x, \ i, j = 0, 1, \dots\}.$$

we constructed the following difference scheme for Problem (3.3)

$$A_i y_{i-1}^{j+1} - C_i y_i^{j+1} + B_i y_{i+1}^{j+1} = -F_i^j, \quad i = 1, 2, \dots, \tag{3.4}$$

$$y_0^{j+1} = \alpha_1 y_1^{j+1} + \beta_1^j, \tag{3.4a}$$

$$y_i^{j+1} \to 0, \ i \to \infty, \ j = 0, 1, 2, \dots,$$

$$y_i^0 = \begin{cases} Q/(u_k h_z), & i = k, \\ 0, & i \neq k, \end{cases} \tag{3.5}$$

where

$$\begin{aligned} &A_i = \rho \chi_i a_i, \quad B_i = \rho \chi_i a_{i+1} + \rho b_i a_{i+1} h_z, \\ &C_i = A_i + B_i + u_i + \sigma h_x, \quad F_i = u_i y_i^j, \\ &\rho = h_x / h_z^2, \quad k = [H/h_z], \\ &\alpha_1 = \frac{A_0 + B_0}{C_0 + 2\alpha h_z A_0}, \quad \beta_1 = \frac{F_0}{C_0 + 2\alpha h_z A_0}, \end{aligned} \tag{3.6}$$

and the quantities a_i, b_i, u_i, χ_i are defined in [4, 5].

Note that (3.5) is obtained by integration of the initial condition in (3.3a) over the interval $(z_i - 0.5h_z, z_i + 0.5h_z)$. Equation (3.4) may be written in the form

$$\hat{y}_i = p_i \hat{y}_{i-1} + q_i \hat{y}_{i+1} + r_i \quad (i = 0, 1, \dots), \tag{3.7}$$

where $\hat{y}$ stands for y^{j+1},

$$\begin{aligned} &p_0 = 0, \quad q_0 = \alpha_1, \quad r_0 = \beta_1, \\ &p_i = \frac{A_i}{C_i}, \quad q_i = \frac{B_i}{C_i}, \quad r_i = \frac{F_i}{C_i}, \quad (i = 1, 2, \dots). \end{aligned} \tag{3.8}$$

There have been established the following result:

Theorem 3.1. *Assume that one of the following conditions is satisfied:*

a) $\dfrac{u_i}{a_i} \to L \neq 0$ *as* $i \to \infty$,

b) $\dfrac{u_i}{a_i} \to \infty$ *as* $i \to \infty$.

Then,

i) the difference scheme (3.7) - (3.8) has the unique solution, which is nonnegative and for each j $(j = 0, 1, 2, \dots)$ *monotonously tends to zero,*

ii) the scheme is unconditionally stable and there is the estimate

$$\|y^{j+1}\| \leq \|y^0\|, \tag{3.9}$$

where $\|y^j\| = \sup_{i\geq 0} |y_i^j|$.

In addition to the above result we shall obtain some new properties of the solution of (3.7) - (3.8).

For this we need the following

Lemma 3.1. *Let the infinite system*

$$x_i = \sum_{k=1}^{\infty} c_{ik} x_k + b_i, \quad c_{ik} \geq 0, \ b_i \geq 0,$$

$$X_i = \sum_{k=1}^{\infty} C_{ik} X_k + B_i, \quad C_{ik} \geq 0, \ B_i \geq 0, \ (i, k = 1, 2, \dots)$$

have the unique bounded nonnegative solution.

If

$$c_{ik} \leq C_{ik}, \ b_i \leq B_i, \ i, k = 1, 2, \dots,$$

then

$$x_i \leq X_i, \ i = 1, 2, \dots.$$

Proof. The assertion follows from the theorem on existence of solution of an system via dominating system in [6].

Having in mind Theorem 3.1 and applying Lemma 3.1 to the system (3.1) with different values of α and σ we get the following

Theorem 3.2. *If* α *or* σ *increases then the solution of (3.7) - (3.8) decreases.*

This conclusion completely fits to physical picture of the problem, namely, from increasing of the coefficient of conversion and coefficient of absorption of the bedding surface $z = 0$ follows decreasing of the concentration of the pollutant in the atmosphere.

Now we shall compare the solution of (3.7) - (3.8) with the solutions of the problems with other boundary conditions.

First, let us consider the problem in a layer $z \leq \mathcal{H}$ with the boundary condition

$$\frac{\partial \varphi}{\partial z} = 0\,, \quad z = \mathcal{H}\,, \tag{3.10}$$

or

$$\varphi = 0\,, \quad z = \mathcal{H}\,, \tag{3.11}$$

and the boundary condition on $z = 0$ being the same as in (3.3).

Assume that $\mathcal{H} = Nh_z$.

As for the boundary surface $z = 0$ we suppose that the differential equation (3.3) is valid inclusively on the boundary $z = \mathcal{H}$ i.e. the difference equation (3.4) is true for $i = N$ inclusively

$$A_N \hat{y}_{N-1} - C_N \hat{y}_N + B_N \hat{y}_{N+1} = -F_N\,. \tag{3.12}$$

For the approximation of (3.10) with second order accuracy we use the centered difference derivative. In result we get $\hat{y}_{N+1} = \hat{y}_{N-1}$. Inserting this into (3.12) we get

$$\hat{y}_N = p_N \hat{y}_{N-1} + r_N\,,$$

where

$$p_N = \frac{A_N + B_N}{C_N}\,, \quad r_N = \frac{F_N}{C_N}\,.$$

Thus, the solution Y_i^j $(i = \overline{0, N},\ j = 0, 1, \ldots)$ of the problem with the boundary condition (3.10) will satisfy the system

$$\begin{aligned} \widehat{Y}_i &= P_i \widehat{Y}_{i-1} + Q_i \widehat{Y}_{i+1} + R_i\,, \quad i = \overline{0, N-1}\,, \\ \widehat{Y}_N &= P_N \widehat{Y}_{N-1} + R_N\,, \end{aligned} \tag{3.13}$$

where

$$P_0 = 0\,,\ Q_0 = \alpha_1\,,\ R_0 = \beta_1\,,$$
$$P_i = \frac{A_i}{C_i}\,,\ Q_i = \frac{B_i}{C_i}\,,\ R_i = \frac{F_i}{C_i}\,,\ (i = \overline{1, N-1})\,,$$
$$P_N = \frac{A_N + B_N}{C_N}\,,\ R_N = \frac{F_N}{C_N}\,. \tag{3.14}$$

At the same time, denoting by $\mathcal{Y}_i^j$ $(i = \overline{0, N},\ j = 0, 1, \dots)$ the solution of the problem with (3.11) we have

$$\begin{aligned} \widehat{\mathcal{Y}}_i &= P_i \widehat{\mathcal{Y}}_{i-1} + Q_i \widehat{\mathcal{Y}}_{i+1} + R_i\,,\ i = \overline{0, N-1}\,, \\ \widehat{\mathcal{Y}}_N &= 0\,. \end{aligned} \tag{3.15}$$

Adding $\widehat{Y}_i = 0$ and $\widehat{\mathcal{Y}}_i = 0$ for $i \geq N+1$ to (3.13) and (3.15) respectively and applying Lemma 3.1 with preliminary convincing of the existence of the unique bounded nonnegative solutions of these systems we get

Lemma 3.2. *For the solutions $\widehat{Y}_i$ and $\widehat{\mathcal{Y}}_i$ of (3.13) and (3.15) respectively there holds the relation*

$$\widehat{Y}_i \leq \widehat{\mathcal{Y}}_i \quad (i = \overline{0, N},\ j = 0, 1, \dots)\,.$$

Now we compare $\widehat{Y}_i$ with the solution $\hat{y}_i$ of (3.7) - (3.8).

According to Theorem 3.1 we have $\hat{y}_{N+1} < \hat{y}_{N-1}$. Hence $\hat{y}_{N+1} = \tilde{p}\hat{y}_{N-1}$ with $\tilde{p} < 1$ and we can rewrite (3.7) for $i = N$ in the form $\hat{y}_N = \tilde{p}_N \hat{y}_{N-1} + r_N$, where $\tilde{p}_N = p_N + \tilde{p} q_N$.

Taking into account (3.8) and (3.14) we have $\tilde{p}_N < P_N$. Arguing similarly as in obtaining Lemma 3.2 we arrive at

Theorem 3.3. *For the approximate solutions $\mathcal{Y}_i^j$, y_i^j and Y_i^j of Problem (3.3) with one of the following boundary conditions*

$$\varphi = 0\,,\ z = \mathcal{H}\,,$$
$$\varphi = 0\,,\ z \to \infty\,,$$
$$\frac{\partial \varphi}{\partial z} = 0\,,\ z = \mathcal{H}\,,$$

respectively, there hold relations

$$\mathcal{Y}_i^j \leq y_i^j \leq Y_i^j \quad (i = \overline{0, N},\ j = 0, 1, \dots)\,.$$

Remark. The above result can be also obtained by using corollaries of the maximum principle for finite difference scheme (see [7]).

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* *Institute of Information Technology*
NCST of Vietnam
Hanoi, Vietnam.

** *Institute of Mechanics*
NCST of Vietnam
Hanoi, Vietnam.