On the numerical solution of some problems of environmental pollution

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Abstract. 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 to plants, animals and humans. Therefore, the development of industry must be coupled with the protection of the environment. In this connection we shall consider the problems of optimal location of industrial enterprises and optimization of emissions from enterprises for ensuring sanitary environment criteria. Moreover, we study the problem of determination of the coefficients of diffusion and the coefficient of transformation of aerosols. Several numerical experiments illustrate the ability of the presented methods.

1 Introduction

At the beginning of this chapter will give a brief introduction to the mathematical formulation of air pollution models. Let G be a cylindrical domain in the three–dimensional space with the side surface Σ, the upper surface Σ_H $(z = H)$ and the bottom surface Σ_0 $(z = 0)$. In the sequel we shall use the following notations:

- $\varphi(x, y, z, t)$ denotes the concentration of aerosol pollutants
- $\mathbf{u} = u\mathbf{i} + v\mathbf{j} + w\mathbf{k}$ is the velocity vector of wind
- $\sigma \geq 0$ stands for the transformation coefficient of pollutants
- μ, ν are the horizontal and vertical coefficients of diffusion, respectively
- Σ_- and Σ_+ are the parts of the side surface Σ, where $u_n = \mathbf{u} \cdot \mathbf{n} < 0$ and $u_n \geq 0$, respectively. Here, $\mathbf{n}$ is the outward unit normal to Σ
- $w_g = \mathrm{constant} > 0$ denotes the falling velocity of the pollutants by gravity
- f is the power of the source.

The problem of air pollution is stated as follows: Determine the function $\varphi(x,y,z,t)$ that satisfies the differential equation

$$\frac{\partial\varphi}{\partial t}+u\frac{\partial\varphi}{\partial x}+v\frac{\partial\varphi}{\partial y}+(w-w_g)\frac{\partial\varphi}{\partial z}-\mu(\frac{\partial^2\varphi}{\partial x^2}+\frac{\partial^2\varphi}{\partial y^2})-\frac{\partial}{\partial z}(\nu\frac{\partial\varphi}{\partial z})+\sigma\varphi=f, \tag{1}$$

and the following initial and boundary conditions

$$\begin{aligned}\varphi&=\varphi_0 \quad \text{at} \quad t=0,\\ \frac{\partial\varphi}{\partial z}&=\alpha\varphi \quad \text{on} \quad \Sigma_0,\\ \frac{\partial\varphi}{\partial z}&=0 \quad \text{on} \quad \Sigma_H,\\ \varphi&=\varphi_s \quad \text{on} \quad \Sigma_-,\\ \frac{\partial\varphi}{\partial \mathbf{n}}&=0 \quad \text{on} \quad \Sigma_+.\end{aligned} \tag{2}$$

Moreover, we assume here that (cf. [13])

$$\begin{aligned}\operatorname{div}\mathbf{u}=\frac{\partial u}{\partial x}+\frac{\partial v}{\partial y}+\frac{\partial w}{\partial z}=0,\\ w=0 \quad \text{at} \quad z=0,\, z=H.\end{aligned} \tag{3}$$

Using the first relation in (3) and considering $w-w_g$ as the vertical component of the vector $\mathbf{u}$ with the notation $\Delta\varphi=\frac{\partial^2\varphi}{\partial x^2}+\frac{\partial^2\varphi}{\partial y^2}$ we can rewrite the equation (1) in the form

$$\frac{\partial\varphi}{\partial t}+\operatorname{div}(\mathbf{u}\varphi)-\mu\Delta\varphi-\frac{\partial}{\partial z}(\nu\frac{\partial\varphi}{\partial z})+\sigma\varphi=f. \tag{4}$$

Instead of the two boundary conditions on two parts of Σ it is possible to pose the following one

$$\varphi=\varphi_s \quad \text{on} \quad \Sigma. \tag{5}$$

We shall refer to the equation (1) as the *main equation* and to the problem (1), (2) or (1), (5) as the *main problems*. It is well–known that the above problems allow for a unique solution.

The problem (1), (2) is a general 3D one. In many cases it is useful to use a 2D model that is an adequate approximation of the 3D problem:

$$\begin{aligned}\frac{\partial\varphi}{\partial t}+u\frac{\partial\varphi}{\partial x}+v\frac{\partial\varphi}{\partial y}-\mu\Delta\varphi+\sigma\varphi=f \quad &\text{in} \quad \Omega,\\ \varphi=\varphi_0 \quad &\text{at} \quad t=0,\\ \varphi=\varphi_s \quad \text{on} \quad \Gamma \quad &\text{at} \quad u_n<0,\\ \frac{\partial\varphi}{\partial \mathbf{n}}=0 \quad \text{on} \quad \Gamma \quad &\text{at} \quad u_n\geq 0,\end{aligned} \tag{6}$$

where Γ is the boundary of the 2D domain Ω. Here it is assumed that the components of velocity u and v do not change with the altitude in the active layer of the substance transport and diffusion. In the above equation $\varphi(x, y, t)$ is the average of the concentration of pollutants in all heights of the cylindrical domain under consideration.

Many practical problems, for example, the substance (e.g. saline and alum) propagation in rivers (see [3], [16]), the stationary problem of air pollution generated by a point source (see [4], [15]) can even be reduced to the following 1D problem:

$$\begin{aligned} \frac{\partial \varphi}{\partial t} + u\frac{\partial \varphi}{\partial x} - \mu\frac{\partial^2 \varphi}{\partial x^2} + \sigma\varphi = f, \quad -\infty < x < +\infty,\ t > 0, \\ \varphi = \varphi_0 \quad \text{at} \quad t = 0, \\ \varphi \to 0 \quad \text{as} \quad |x| \to \infty. \end{aligned} \tag{7}$$

If we limit the problem to a finite interval then we can pose the following boundary conditions

$$\begin{aligned} \varphi = \varphi_s \quad \text{at} \quad B_-, \\ \frac{\partial \varphi}{\partial x} = 0 \quad \text{at} \quad B_+, \end{aligned}$$

where B_- and B_+ denote the endpoints at which the flow comes in and comes out, respectively.

2 Adjoint problems

In this section we consider the main problem (1), (2) with homogeneous initial and boundary conditions, i.e. the problem

$$\begin{aligned} \frac{\partial \varphi}{\partial t} + \operatorname{div}(\mathbf{u}\varphi) - \mu\Delta\varphi - \frac{\partial}{\partial z}(\nu\frac{\partial \varphi}{\partial z}) + \sigma\varphi = f, \\ \varphi = 0 \quad \text{at} \quad t = 0, \\ \frac{\partial \varphi}{\partial z} = \alpha\varphi \quad \text{on} \quad \Sigma_0, \\ \frac{\partial \varphi}{\partial z} = 0 \quad \text{on} \quad \Sigma_H, \\ \varphi = 0 \quad \text{on} \quad \Sigma_-, \\ \frac{\partial \varphi}{\partial \mathbf{n}} = 0 \quad \text{on} \quad \Sigma_+. \end{aligned} \tag{8}$$

By the same way as in [13], [14] for the main problem with homogeneous boundary conditions and a periodic condition in the time variable we obtain the adjoint problem

$$\begin{aligned} -\frac{\partial \varphi^*}{\partial t} - \operatorname{div}(\mathbf{u}\varphi^*) - \mu\Delta\varphi^* - \frac{\partial}{\partial z}(\nu\frac{\partial \varphi^*}{\partial z}) + \sigma\varphi^* = p, \\ \varphi^* = 0 \quad \text{at} \quad t = T, \\ \frac{\partial \varphi^*}{\partial z} = \alpha\varphi^* \quad \text{on} \quad \Sigma_0, \\ \frac{\partial \varphi^*}{\partial z} = 0 \quad \text{on} \quad \Sigma_H, \\ \varphi^* = 0 \quad \text{on} \quad \Sigma_-, \\ \mu\frac{\partial \varphi^*}{\partial \mathbf{n}} + u_n\varphi^* = 0 \quad \text{on} \quad \Sigma_+. \end{aligned} \tag{9}$$

Here, the *complementary conditions* (3) are used. There is the following adjoint relation

$$\int_0^T dt \int_G p\varphi dG = \int_0^T dt \int_G \varphi^* f dG. \tag{10}$$

Similarly to the 3D case we consider the 2D problem with homogeneous initial and boundary conditions

$$\begin{aligned} \frac{\partial \varphi}{\partial t} - \operatorname{div}(\mathbf{u}\varphi) - \mu\Delta\varphi + \sigma\varphi = f, \\ \varphi = \varphi_0 \quad \text{at} \quad t = 0, \\ \varphi = \varphi_s \quad \text{on} \quad \Gamma \quad \text{at} \quad u_n < 0, \\ \frac{\partial \varphi}{\partial \mathbf{n}} = 0 \quad \text{on} \quad \Gamma \quad \text{at} \quad u_n \geq 0. \end{aligned} \tag{11}$$

The adjoint problem for the above problem reads

$$\begin{aligned} -\frac{\partial \varphi^*}{\partial t} - \operatorname{div}(\mathbf{u}\varphi^*) - \mu\Delta\varphi^* + \sigma\varphi^* = p, \\ \varphi^* = 0 \quad \text{at} \quad t = T, \\ \varphi^* = \varphi_s^* \quad \text{on} \quad \Gamma \quad \text{at} \quad u_n < 0, \\ \mu\frac{\partial \varphi^*}{\partial \mathbf{n}} + u_n\varphi^* = 0 \quad \text{on} \quad \Gamma \quad \text{at} \quad u_n \geq 0, \end{aligned} \tag{12}$$

and the adjoint relation has the form

$$\int_0^T \int_\Omega p\varphi dG = \int_0^T dt \int_\Omega \varphi^* f d\Omega. \tag{13}$$

In the 1D case for the main problem with homogeneous initial and boundary conditions

$$\begin{aligned} \frac{\partial \varphi}{\partial t} + u\frac{\partial \varphi}{\partial x} - \mu\frac{\partial^2 \varphi}{\partial x^2} + \sigma\varphi = f, \quad a < x < b,\ t > 0, \\ \varphi = 0 \quad \text{at} \quad B_-, \\ \frac{\partial \varphi}{\partial x} = 0 \quad \text{at} \quad B_+, \end{aligned} \tag{14}$$

the adjoint problem reads

$$
\begin{aligned}
-\frac{\partial\varphi^*}{\partial t} - u\frac{\partial\varphi^*}{\partial x} - \mu\frac{\partial^2\varphi^*}{\partial x^2} + \sigma\varphi^* = p, \quad a < x < b,\\
\varphi^* = 0 \quad \text{at} \quad t = T,\\
\varphi^* = 0 \quad \text{at} \quad B_-,\\
\mu\frac{\partial\varphi^*}{\partial x} + u\varphi^* = 0 \quad \text{at} \quad B_+.
\end{aligned}
\tag{15}
$$

If the 1D main problem is considered in the unbounded domain $-\infty < x < +\infty$ with the decay condition $\varphi \to 0$ for $|x| \to \infty$, then its adjoint problem is

$$
\begin{aligned}
-\frac{\partial\varphi^*}{\partial t} - u\frac{\partial\varphi^*}{\partial x} - \mu\frac{\partial^2\varphi^*}{\partial x^2} + \sigma\varphi^* = p, \quad -\infty < x < +\infty,\\
\varphi^* = 0 \quad \text{at} \quad t = T,\\
\varphi^* \to 0 \quad \text{at} \quad |x| \to \infty.
\end{aligned}
\tag{16}
$$

It is important to remark that all the stated adjoint problems can be reduced to the corresponding problems by making the substitution $t' = T - t$ and $\mathbf{u}' = -\mathbf{u}$. Therefore, all the qualitative results such as the uniqueness of solution for the main problems are also valid for the adjoint ones and all numerical methods for solving main problems are also applicable to adjoint problems.

3 Numerical solution of main and adjoint problems

For solving the main and adjoint problems of aerosol propagation there exists a large number of numerical schemes. Mainly, they are based on splitting methods developed by Yanenko [22] and Marchuk [13]. These schemes are stable and possess good approximation properties, but they may lead to solutions with negative values that are meaningless. Therefore, it is desired to construct difference schemes that avoid this defect. These difference schemes must ensure that if all initial and boundary conditions are nonnegative, then the solution of the corresponding problem is nonnegative, too. The difference schemes of this type are called *monotone* (or *positive*) ones (see [7]). Below, we present the method for constructing monotone difference schemes for the main problem (1), (2) developed in [6], [5]. Throughout this chapter we shall use the standard difference notations of Samarskii [17].

We begin with the consideration of the 1D parabolic problem

$$
\begin{aligned}
c(x,t)\frac{\partial\varphi}{\partial t} = L\varphi + f(x,t), \quad 0 < x < 1,\ 0 < t \le T,\\
\varphi(0,t) = \mu_1(t), \quad \varphi(1,t) = \mu_2(t),\\
\varphi(x,0) = \varphi_0(x),
\end{aligned}
\tag{17}
$$

where

$$
\begin{gathered}
L\varphi = \frac{\partial}{\partial x}(k(x,t)\frac{\partial \varphi}{\partial x}) + r(x,t)\frac{\partial \varphi}{\partial x} - q(x,t)\varphi, \\
0 < c_1 \le k(x,t) \le c_2,\ c(x,t) \ge c_1,\ q(x,t) \ge 0.
\end{gathered} \tag{18}
$$

We will construct a difference scheme for this problem on the uniform grid

$$
\omega_{h\tau} = \{x_i = ih, t_j = j\tau, i = 0,1,\ldots,N; j = 0,1,\ldots,J; h = 1/N; \tau = T/J\}.
$$

Firstly, we associate with the operator L a perturbation operator

$$
\tilde{L}\varphi = \chi\frac{\partial}{\partial x}(k(x,t)\frac{\partial \varphi}{\partial x}) + r(x,t)\frac{\partial \varphi}{\partial x} - q(x,t)\varphi, \tag{19}
$$

where $\chi = 1/(1+R)$, $R = 0.5h|r|/k$ and approximate the latter one by the difference operator

$$
\tilde{\Lambda}y = \chi(ay_{\bar{x}})_x + b^+a^{(+1)}y_x + b^-ay_{\bar{x}} - dy, \tag{20}
$$

where

$$
\begin{gathered}
b^{\pm} = \tilde{r}^{\pm}(x,t), \quad a = k(x-0.5h,t), \quad d = q(x,t), \\
r^{\pm} = (r \pm |r|)/2, \quad \tilde{r}^{\pm} = r^{\pm}/k, \quad a_i^{(+1)} = a_{i+1}.
\end{gathered}
$$

Next, the problem (17) is replaced by the difference scheme

$$
\begin{aligned}
c(x,\bar{t})y_t &= \tilde{\Lambda}(\bar{t})\hat{y} + f, \quad \bar{t} = t + \tau/2, \\
y(0,t) &= \mu_1(t), \quad y(1,t) = \mu_2(t), \\
y(x,0) &= \varphi_0(x).
\end{aligned} \tag{21}
$$

This scheme has a truncation error of order $\mathrm{O}(h^2+\tau)$ and is monotone. In this aspect the Crank–Nicolson difference scheme for the problem (17) is not better than (21) although it is of order $\mathrm{O}(h^2+\tau^2)$ because the Crank–Nicolson method is monotone only if $\tau/h^2 \le 1/(2\min k + h\max|r|)$. The same conclusion holds for the so–called *optimal weighting scheme* of Wang and Lacroix [21].

If instead of a Dirichlet boundary condition there are Robin boundary conditions posed at the endpoints, for example,

$$
\big(\alpha\varphi + \frac{\partial \varphi}{\partial x}\big)(1,t) = \mu_2(t),
$$

then using the difference boundary condition

$$
\alpha\varphi_N + \frac{y_{N+1} - y_{N-1}}{2h} = \mu_2,
$$

we also obtain a monotone difference scheme for the corresponding differential problem.

Now, we consider the three–dimensional problem for the main problem (1), (2). For simplicity we suppose that the domain G is a parallelepiped $[0, X] \times [0, Y] \times [0, Z]$. In order to construct a difference scheme for (1), (2) we rewrite equation (1) in a convenient form

$$\frac{\partial \varphi}{\partial t} - (L_1 + L_2 + L_3)\varphi = f \quad \text{in} \quad G \times (0, T], \tag{22}$$

where

$$\begin{aligned} L_1\varphi &= \mu \frac{\partial^2 \varphi}{\partial x^2} - u\frac{\partial \varphi}{\partial x}, \\ L_2\varphi &= \mu \frac{\partial^2 \varphi}{\partial y^2} - v\frac{\partial \varphi}{\partial y}, \\ L_3\varphi &= \frac{\partial}{\partial z}(\nu \frac{\partial \varphi}{\partial z}) - (w - w_g) - \sigma\varphi. \end{aligned} \tag{23}$$

We employ on the domain G the uniform grid $G_h = \{x_i = ih_1, y_j = jh_2, z_k = kh_3\}$ and approximate the above differential operators (23) by the following monotone difference operators

$$\begin{aligned} \tilde{\Lambda}_1\phi &= \chi^{(x)}\mu\phi_{\bar{x}x} - u\phi_{\bar{x}}, \\ \tilde{\Lambda}_2\phi &= \chi^{(y)}\mu\phi_{\bar{y}y} - v\phi_{\bar{y}}, \\ \tilde{\Lambda}_3\phi &= \chi^{(z)}(a\phi_{\bar{z}})_z + b^+a^{(+1)}\phi_x + b^- a\phi_{\bar{x}} - \sigma\phi, \end{aligned}$$

where

$$\begin{aligned} \chi^{(x)} &= 1/(1 + R^{(x)}), \quad R^{(x)} = 0.5h_1u/\mu, \\ \chi^{(y)} &= 1/(1 + R^{(y)}), \quad R^{(y)} = 0.5h_2v/\mu, \\ \chi^{(z)} &= 1/(1 + R^{(z)}), \quad R^{(z)} = 0.5h_3|r|/\nu, \quad r = w - w_g, \\ a &= \nu(z - 0.5h_3), \quad a_i^{(+1)} = a_{i+1}, \quad b^{\pm} = r^{\pm}/\nu, \quad r^{\pm} = (r \pm |r|)/2. \end{aligned}$$

Now we write the difference scheme for the equation (22) with the boundary conditions for the case that the wind velocity is given by $\mathbf{u} = (u, 0, 0)$:

$$\begin{aligned} &\frac{\phi^{l+1/3} - \phi^l}{\tau} - \tilde{\Lambda}_1\phi^{l+1/3} = 0, \quad \phi_0^{l+1/3} = 0, \quad \phi_{I+1}^{l+1/3} - \phi_{I-1}^{l+1/3} = 0, \\ &\frac{\phi^{l+2/3} - \phi^{l+1/3}}{\tau} - \tilde{\Lambda}_2\phi^{l+2/3} = 0, \quad \phi_0^{l+2/3} = 0, \quad \phi_J^{l+2/3} = 0, \\ &\frac{\phi^{l+1} - \phi^{l+2/3}}{\tau} - \tilde{\Lambda}_3\phi^{l+1} = f^{l+1}, \quad \alpha\phi_0^{l+1} - \frac{\phi_1^{l+1} - \phi_{-1}^{l+1}}{2h_3} = 0, \quad \phi_K^{l+1} = 0, \\ &l = 0, 1, \ldots \end{aligned} \tag{24}$$

Here, for brevity, we write only one space index for the computation direction, omitting other indexes, for example ϕ_I stands for ϕ_{Ijk}.

Due to the monotonicity of each component difference scheme in (24) it is possible to prove the positiveness of the solution of (24), its stability and the convergence order $\mathrm{O}(h^2 + \tau)$. Finally, we note that we considered in [15] another finite difference scheme based on the *Abrashin alternative directions technique* [1].

It should be remarked that, as many authors, we consider problems of propagation of pollutants in large bounded domains and put conditions on its boundary. These conditions indeed are artificial and close to real conditions. In the 1D case in [7] we have constructed and studied monotone difference schemes for air pollution problems on unbounded domains using *transparent boundary conditions* (TBC). This (discrete) TBC method was developed by Ehrhardt for 1D parabolic problems [9], [10].

Numerical Example. In order to test the above proposed difference method we consider the equation (1) with $f = \delta(x_0, y_0, H)q(t)$, $\sigma = 0$, $\mathbf{u} = (u, 0, 0), w_g = 0$ and the following initial and boundary conditions

$$\begin{aligned} \varphi = 0 &\quad \text{at} \quad t = 0, \\ \varphi \to 0 &\quad \text{as} \quad x, y \to \pm\infty,\ z \to \infty, \\ \frac{\partial \varphi}{\partial z} = 0 &\quad \text{at} \quad z = 0. \end{aligned}$$

This problem admits the exact solution [12]

$$\varphi = \int_0^t \frac{q(t)}{8\pi^{3/2}\mu\nu^{1/2}} \exp\Big(-\frac{(x - x_0 - u(t-\tau))^2}{4\mu(t-\tau)} - \frac{(y-y_0)^2}{4\mu(t-\tau)} \Big) \Big[\exp\Big(-\frac{(z-H)^2}{4\nu(t-\tau)} \Big) + \exp\Big(-\frac{(z+H)^2}{4\nu(t-\tau)} \Big) \Big] d\tau. \qquad (25)$$

We performed the numerical computation using the difference scheme for the problem with the following data: $\mu = 2$, $\nu = 0.2$, $q(t) = 10$, $u = 2$. We limit the computational domain to $[0, 50] \times [0, 50] \times [0, 10]$ and locate a source at the point $(10, 25, 5)$. Below we present some isograms of concentration of aerosols obtained by the difference scheme and the exact solution.

From the Figures 1–5 one can clearly observe that the numerical solution of the problem (1) in a limited domain agrees well with the analytical solution (25) in the unbounded domain.

For the problem when the source of emission is a point and has a constant power under some assumptions on wind velocity and vertical coefficient of diffusion a monotone difference scheme for unbounded domains was constructed and a high order of accuracy was proven (see [5]).

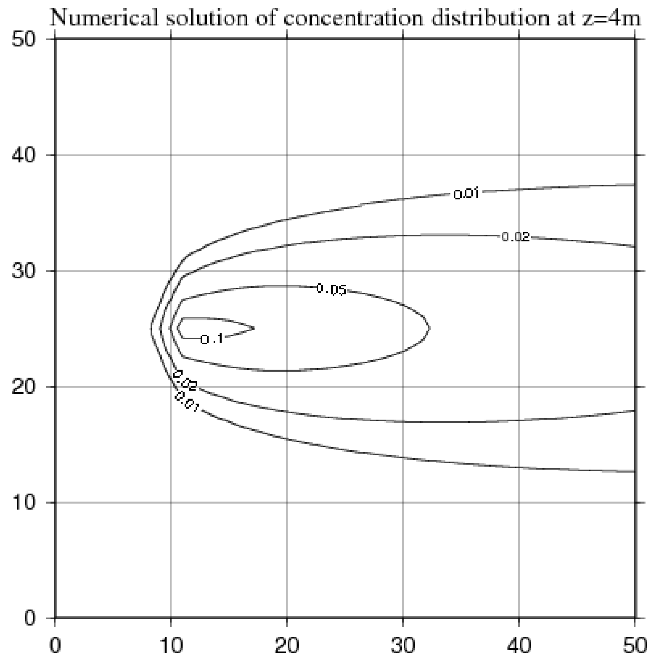

Figure 1: Concentration distribution computed by numerical solution at $z = 4$.

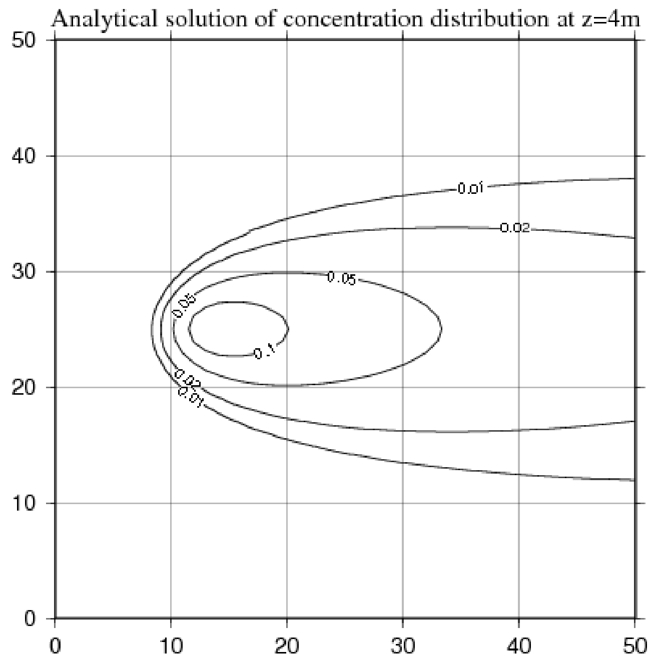

Figure 2: Concentration distribution computed by analytical solution at $z = 4$.

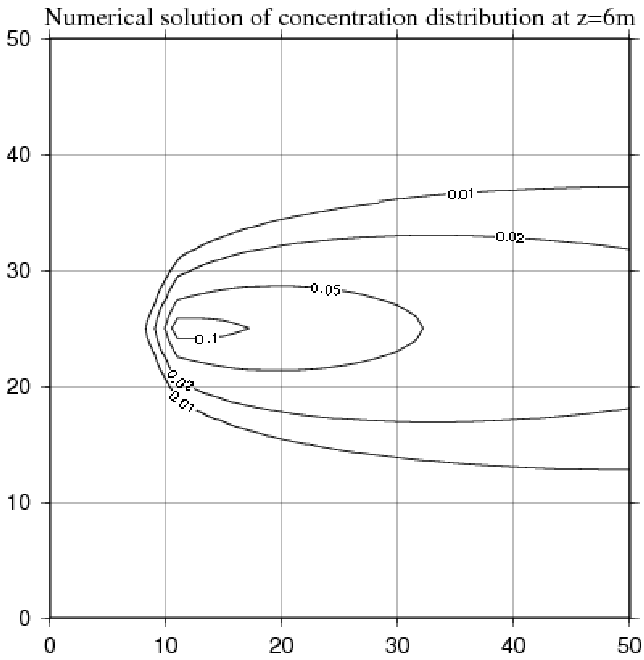

Figure 3: Concentration distribution computed by analytical solution at $z = 6$.

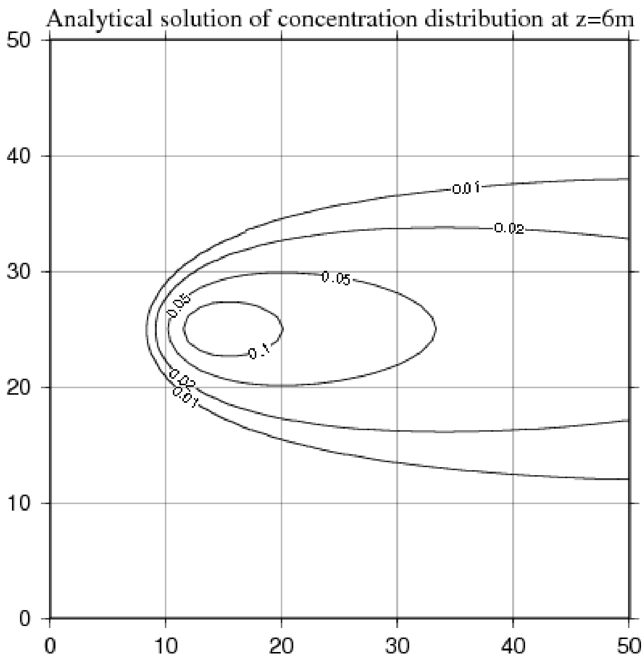

Figure 4: Concentration distribution computed by analytical solution at $z = 6$.

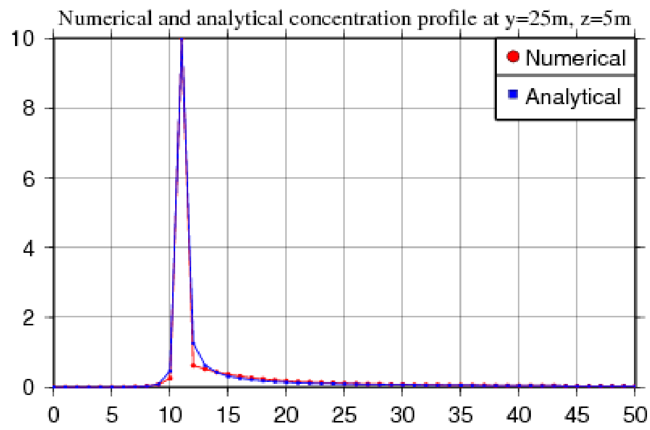

Figure 5: Concentration distribution computed by analytical solution at $y = 25$, $z = 5$.

4 Rational location of industrial plants

First, as in [13], [14], we introduce a functional characterizing the level of pollution in a sensitive area Σ_k on the plane $z = 0$ in the base domain Σ_0

$$J_k = \int_0^T dt \int_{G_k} p_k \varphi dG_k, \tag{26}$$

where G_k is a unit cylinder over the sensitive area Σ_K. In Equation (26) φ denotes, as before, the concentration of pollutants,

$$p_k = \begin{cases} b_k + a_k \delta(z) & \text{in } G_k \\ 0 & \text{outside } G_k \end{cases}. \tag{27}$$

Usually we take

$$b_k = \frac{1}{T}, \quad a_k = w_g + \alpha\nu, \tag{28}$$

where $w_g = \text{constant} > 0$ denotes the falling velocity of the pollutants by gravity. Then

$$\frac{1}{T} \int_0^T dt \int_{G_k} \varphi dG_k \tag{29}$$

is the average amount of aerosols in G_k and

$$\int_0^T dt \int_{G_k} a_k \delta(z) \varphi dG_k = a_k \int_0^T dt \int_{\Sigma_k} \varphi d\Sigma_k \tag{30}$$

is the total fallout of pollutants in the area Σ_k.

Now let there be m *sensitive areas* Σ_k, $k = 1, \dots, m$ on the plane $z = 0$ in the domain Σ_0. These may be populated areas, recreation zones, water reservoirs, etc. We consider the problem of locating a new industrial plant so that the pollution of all the m areas Σ_k does not exceed the approved standards (if such a location is possible in Σ_0 at all). If the location proves impossible on Σ_0 we formulate restrictions on the rate of pollution emissions Q which will make the location of the plant possible.

Suppose that the *approved standards of air pollution* for the sensitive area Σ_k are given by c_k. Then the problem is to choose the position $\mathbf{r_0} = \mathbf{r_0}(x, y, H)$ of the source of aerosol emission such that the conditions

$$J_k \le c_k \quad k = 1, 2, \dots, m \tag{31}$$

are satisfied.

Instead of this problem we can state the problem of finding a position $\mathbf{r_0}$, such that $\max_k J_k$ is minimal, i.e.

$$\min_{\mathbf{r}\in G} \max_k J_k. \tag{32}$$

There may be two methods for solving the above problems.

The first method consists of the following steps:

1. Choose a position $\mathbf{r_0} \in G$
2. Solve the main problem (1), (2) with $f = Q\delta(\mathbf{r} - \mathbf{r_0})$
3. Compute the levels of pollution J_k of the areas Σ_k and verify the conditions (31)

If all the conditions are satisfied then the selected position $\mathbf{r_0}$ may be a location of the source of pollutant emission. Otherwise, choose another $\mathbf{r_0}$ and repeat the above process until a position $\mathbf{r_0}$ satisfies all the conditions.

The described method for solving the problem of plant location requires a great deal of computation due to the solution of many main problems for different test positions $\mathbf{r_0}$, especially if there is a large number of sensitive areas and industrial plants to be constructed. This method in some sense is a ”blind method”. Another method for the plant location problem is to use adjoint problems. Below we describe this method.

Let us represent the solution of the main equation

$$\frac{\partial \varphi}{\partial t} + L\varphi = Q\delta(\mathbf{r} - \mathbf{r_0}),$$

where for short we denote

$$L\varphi = \operatorname{div}(\mathbf{u}\varphi) - \mu\Delta\varphi - \frac{\partial}{\partial z}(\nu\frac{\partial \varphi}{\partial z}) + \sigma\varphi,$$

with the initial and boundary conditions (2) in the form of sum $\varphi = \varphi_1 + \varphi_2$, where φ_1 and

φ_2 are the solutions of the two problems

$$\begin{aligned} \frac{\partial \varphi_1}{\partial t} + L\varphi_1 &= 0, \\ \varphi_1 &= \varphi_0 \quad \text{at} \quad t = 0, \\ \frac{\partial \varphi_1}{\partial z} &= \alpha \varphi_1 \quad \text{on} \quad \Sigma_0, \\ \frac{\partial \varphi_1}{\partial z} &= 0 \quad \text{on} \quad \Sigma_H, \\ \varphi_1 &= \varphi_s \quad \text{on} \quad \Sigma_-, \\ \frac{\partial \varphi_1}{\partial n} &= 0 \quad \text{on} \quad \Sigma_+, \end{aligned} \tag{33}$$

$$\begin{aligned} \frac{\partial \varphi_2}{\partial t} + L\varphi_2 &= Q\delta(\mathbf{r} - \mathbf{r_0}), \\ \varphi_2 &= \varphi_0 \quad \text{at} \quad t = 0, \\ \frac{\partial \varphi_2}{\partial z} &= \alpha \varphi_1 \quad \text{on} \quad \Sigma_0, \\ \frac{\partial \varphi_2}{\partial z} &= 0 \quad \text{on} \quad \Sigma_H, \\ \varphi_2 &= 0 \quad \text{on} \quad \Sigma_-, \\ \frac{\partial \varphi_2}{\partial n} &= 0 \quad \text{on} \quad \Sigma_+. \end{aligned} \tag{34}$$

We remark that the solution φ_1 does not depend on the source of emission while the solution φ_2 depends only on it.

The pollution level functional for a sensitive area Σ_k now is

$$J_k = \int_0^T dt \int_G p_k \varphi dG = \int_0^T dt \int_G p_k \varphi_1 dG + \int_0^T dt \int_G p_k \varphi_2 dG. \tag{35}$$

We denote by φ_{2k}^* the solution of the problem adjoint to (34), namely, the problem

$$\begin{aligned} -\frac{\partial \varphi_{2k}^*}{\partial t} - \operatorname{div}(\mathbf{u}\varphi_{2k}^*) - \mu\Delta\varphi_{2k}^* - \frac{\partial}{\partial z}(\nu \frac{\partial \varphi_{2k}^*}{\partial z}) + \sigma\varphi_{2k}^* &= p_k, \\ \varphi_{2k}^* &= 0 \quad \text{at} \quad t = T, \\ \frac{\partial \varphi_{2k}^*}{\partial z} &= \alpha \varphi_{2k}^* \quad \text{on} \quad \Sigma_0, \\ \frac{\partial \varphi_{2k}^*}{\partial z} &= 0 \quad \text{on} \quad \Sigma_H, \\ \varphi_{2k}^* &= 0 \quad \text{on} \quad \Sigma_-, \\ \mu \frac{\partial \varphi_{2k}^*}{\partial n} + u_n \varphi_{2k}^* &= 0 \quad \text{on} \quad \Sigma_+. \end{aligned} \tag{36}$$

In view of the duality relation

$$\int_0^T dt \int_G p_k \varphi_2 dG = \int_0^T dt \int_G \varphi_{2k}^* Q \delta(\mathbf{r} - \mathbf{r_0}) dG, \tag{37}$$

we obtain

$$J_k = \int_0^T dt \int_G p_k \varphi_1 dG + Q \int_0^T \varphi_{2k}^*(\mathbf{r_0}, t). \tag{38}$$

Thus, in the adjoint approach for calculating the functionals $J_k,\ k = 1, \dots, m$ we have to solve one main problem (33) and m adjoint problems (36) for m sensitive areas. Doing so, the amount of computation is significantly reduced in comparison with the direct approach. This saving of computational effort is a remarkable advantage of the proposed adjoint approach.

In order to choose a suitable position for a plant it is convenient to introduce the following function

$$J(\mathbf{r}) = \max_k J_k(\mathbf{r})$$

and draw isograms of this function.

Numerical Example. In this example we want to study the problem of a plant location with given sensitive areas and approved standards of air pollution. We choose the following parameters:

- domain $G = [0, 1000] \times [0, 1000] \times [0, 50]$ (in meters)
- uniformly grid with step sizes $dx =$ 20m, $dy =$ 20m, $dz =$ 5m
- time of simulation $T = 1000$sec, time step $dt = 5$sec
- velocity vector $\mathbf{u} = (1, -1, 0)$
- falling velocity $w_g = 0.1$
- diffusion coefficients $\mu = 2, \nu = 0.2$
- coefficient of transformation $\sigma = 0$
- source of emission $Q = 50$
- three sensitive areas:
  $\Sigma_1 = [24.5, 27.5]dx \times [8.5, 10.5]dy,$
  $\Sigma_2 = [37.5, 39.5]dx \times [12.5, 14.5]dy,$
  $\Sigma_3 = [29.5, 31.5]dx \times [33.5, 36.5]dy$
- approved standards of air pollution $c_k = 1$, $k = 1, 2, 3$
- initial and boundary conditions are homogeneous.

Below we present in Figures 6–13 isograms of the pollution level functionals $J_k(\mathbf{r})$ for each sensitive area and of the functional $J(\mathbf{r})$ at the heights $z = 30$m and $z = 35$m. Afterwards, we show in Figures 14 and 15 all the places where a plant cannot be located at the heights $z = 30$m and $z = 40$m for the approved standards of air pollution c_k set to unity.

Remark that in this section we consider the problem of rational location of industrial plants in 3D formulation.The 2D and 1D cases were studied by many authors, for example, in [20] its authors found places for locating plants in Halong Bay with the use of 2D model.

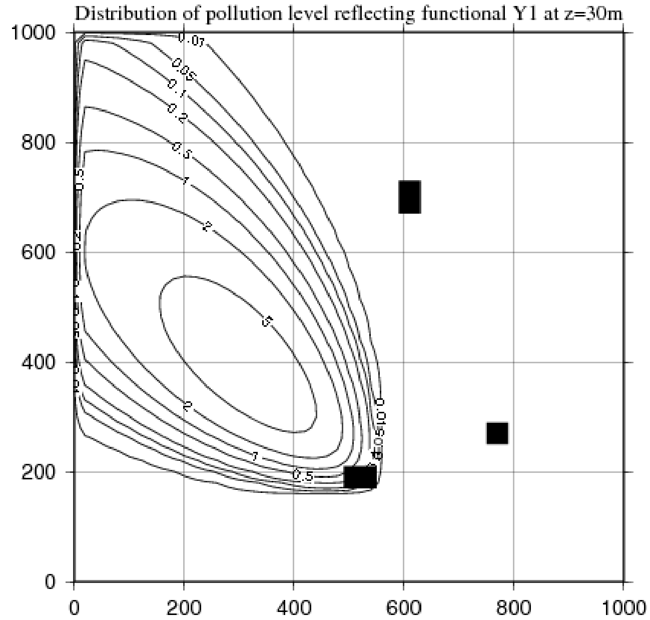

Figure 6: Isogram of pollution level functional J_1 at $z = 30$m.

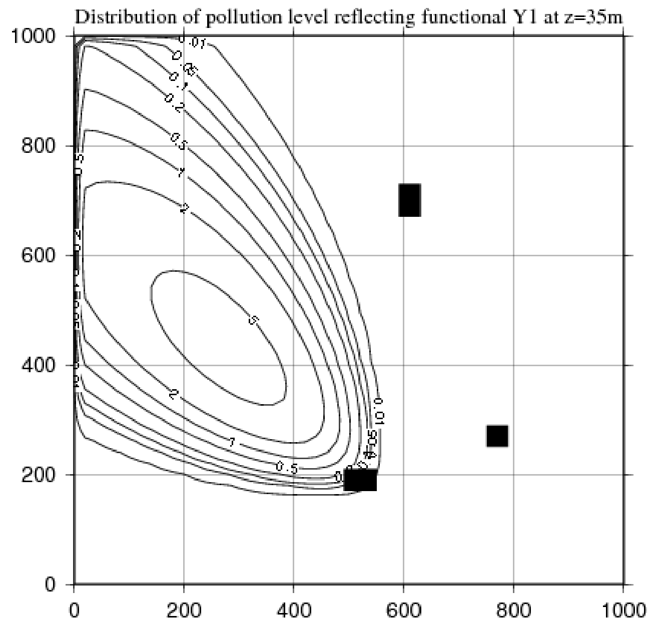

Figure 7: Isogram of pollution level functional J_1 at $z = 35$m.

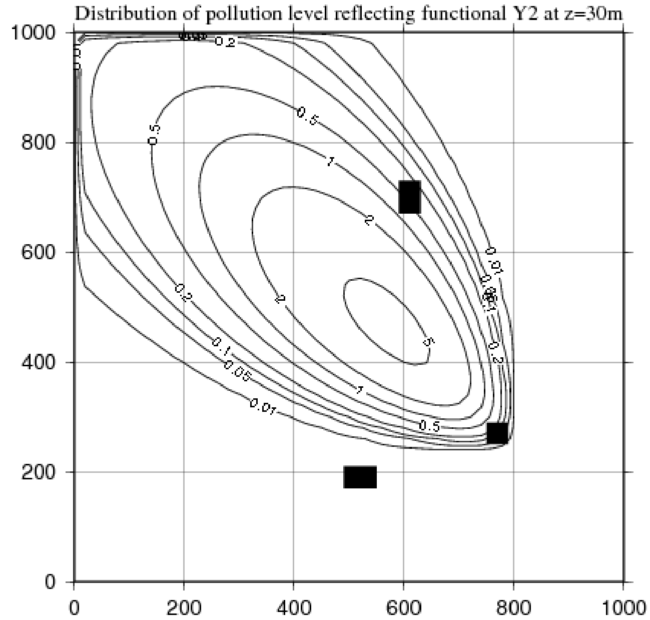

Figure 8: Isogram of pollution level functional J_2 at $z = 30$m.

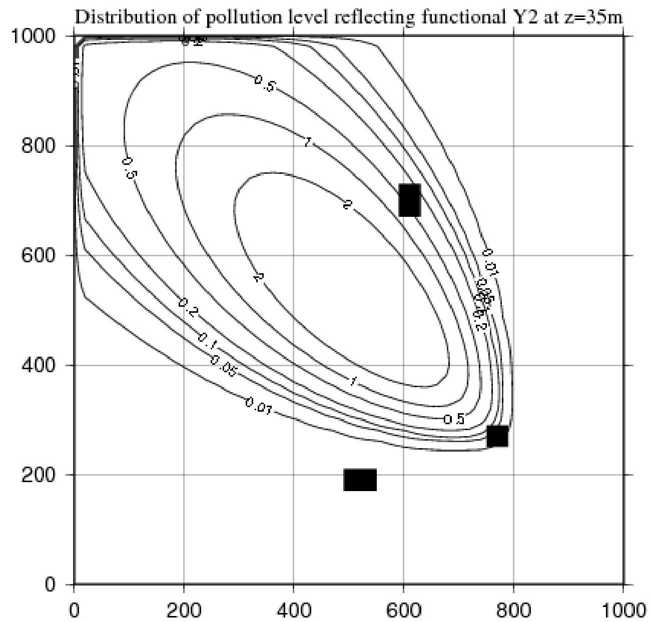

Figure 9: Isogram of pollution level functional J_2 at $z = 35$m.

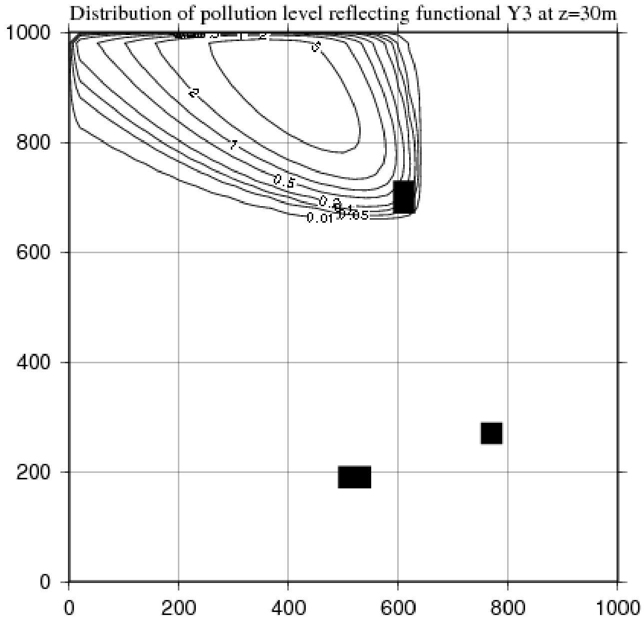

Figure 10: Isogram of pollution level functional J_3 at $z = 30$m.

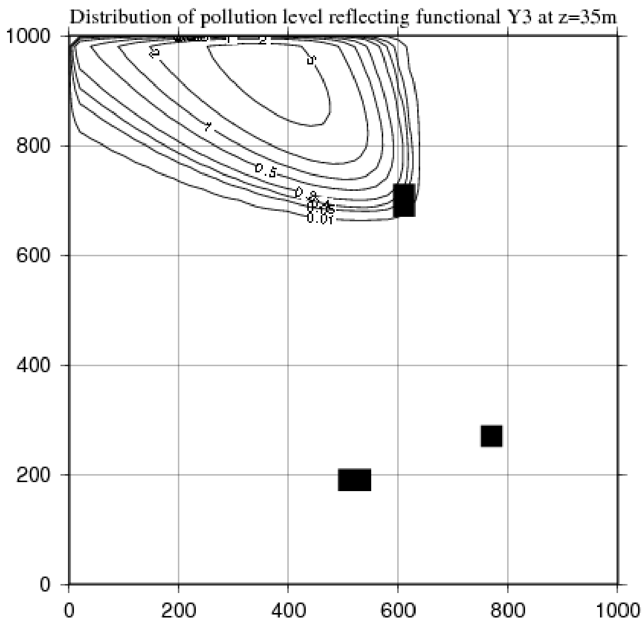

Figure 11: Isogram of pollution level functional J_3 at $z = 35$m.

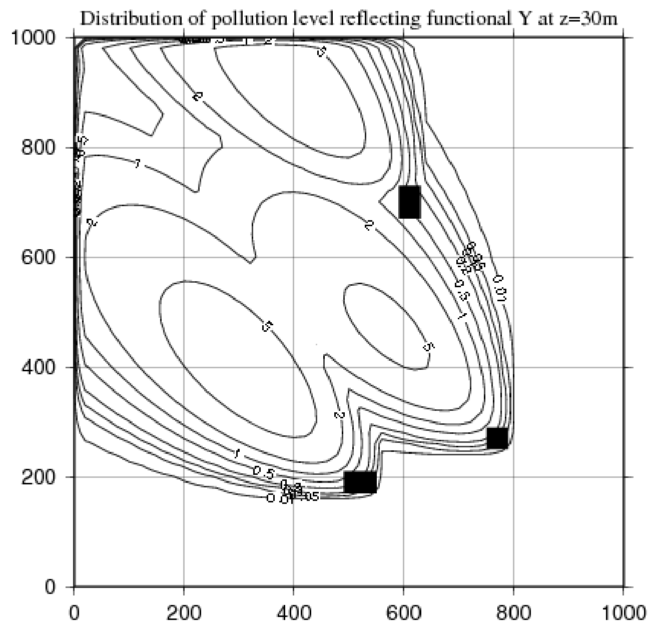

Figure 12: Isogram of pollution level functional J at $z = 30$m.

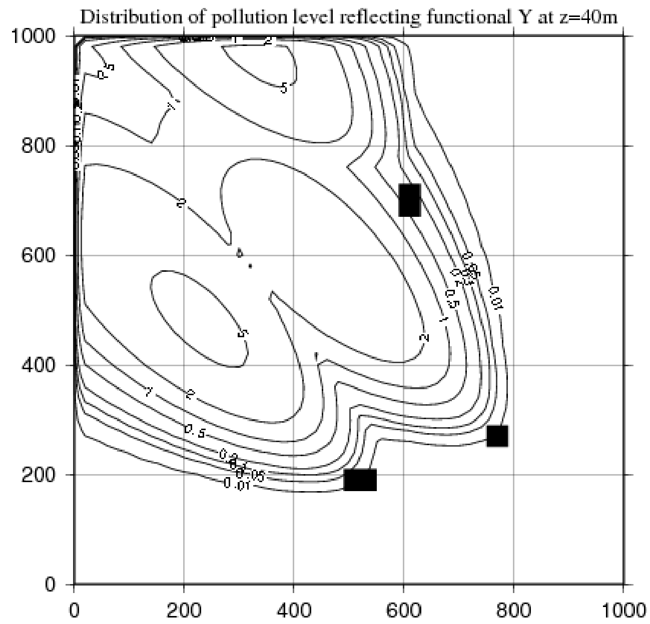

Figure 13: Isogram of pollution level functional J at $z = 40$m.

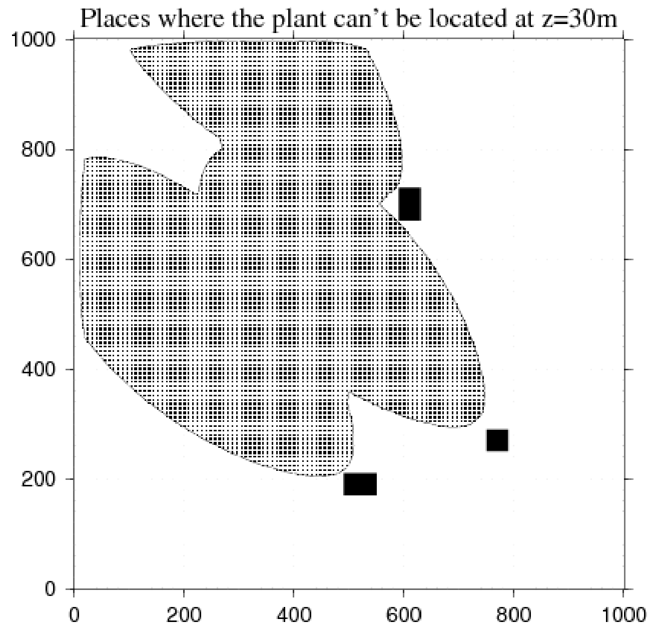

Figure 14: Places where a plant cannot be located at $z = 30$m if $c_1 = c_2 = c_3 = 1$.

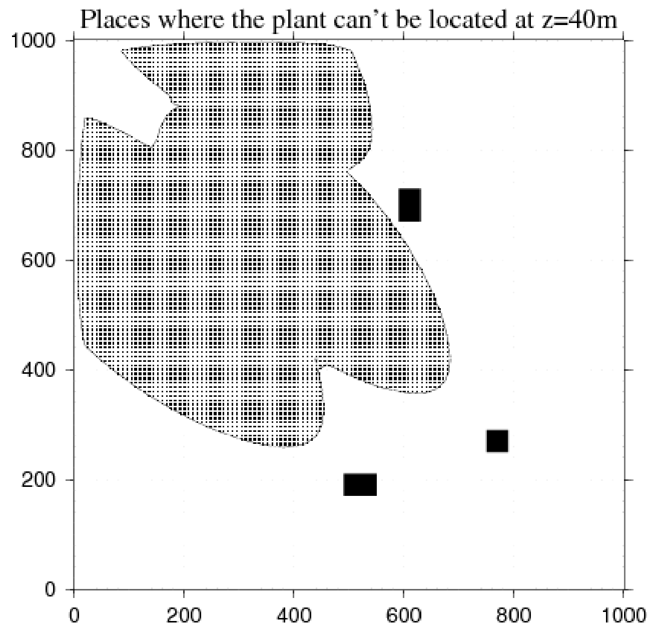

Figure 15: Places where a plant cannot be located at $z = 40$m if $c_1 = c_2 = c_3 = 1$.

A review of 1D problems concerning location of plants and optimization of emissions of operating plants can be found in [8].

5 Optimization of emissions at operating industrial plants

Assume that n plants A_i are located at points $\mathbf{r_i}$, $i = 1, 2, \dots, n$ of a assigned area G. The plants emit $\bar{Q}_i$, $i = 1, \dots, n$ of aerosols per time unit. For simplicity we assume that the emission composition is the same. Furthermore, we suppose that there are m sensitive areas G_k, $k = 1, \dots, m$ to be protected from the polluted aerosols. The task is to determine affordable planned pollution level emissions rate Q_i for every plant so that the pollution level of the sensitive areas do not exceed the standards c_k under the condition that the total investment into technology to keep up the same production level is minimal.

Now we formulate the above problem as a problem of optimization

$$\begin{aligned} I = \sum_{i=1}^{n} \xi_i (\bar{Q}_i - Q_i) \to \min \\ J_k \le c_k, \quad k = 1, 2, \dots, n, \end{aligned} \tag{39}$$

where ξ_i is the cost for reducing emissions per unit of emission rate. The problem (39) may be reduced to a problem of linear programming. Two different approaches are possible: main and adjoint equations.

i) Main equation approach. The main equation of diffusion and transportation of substances emitted by n plants located at the positions $\mathbf{r_i}$ is

$$\begin{aligned} \frac{\partial \varphi}{\partial t} + L\varphi &= \sum_{i=1}^{n} Q_i \delta(\mathbf{r} - \mathbf{r_i}), \\ \varphi &= \varphi_0 \quad \text{at} \quad t = 0, \\ \frac{\partial \varphi}{\partial z} &= \alpha \varphi \quad \text{on} \quad \Sigma_0, \\ \frac{\partial \varphi}{\partial z} &= 0 \quad \text{on} \quad \Sigma_H, \\ \varphi &= \varphi_s \quad \text{on} \quad \Sigma_-, \\ \frac{\partial \varphi}{\partial \mathbf{n}} &= 0 \quad \text{on} \quad \Sigma_+. \end{aligned} \tag{40}$$

We represent the solution of this problem as a superposition of solutions of elementary problems

$$\varphi = \sum_{i=1}^{n} Q_i \varphi_i(\mathbf{r}, t) + \varphi_g, \tag{41}$$

where $\varphi_i(\mathbf{r}, t)$ is a solution to the problem

$$\begin{aligned} \frac{\partial \varphi_i}{\partial t} + L\varphi_i = \delta(\mathbf{r} - \mathbf{r_i}), \\ \varphi_i = 0 \quad \text{at} \quad t = 0, \\ \frac{\partial \varphi_i}{\partial z} = \alpha \varphi_i \quad \text{on} \quad \Sigma_0, \\ \frac{\partial \varphi_i}{\partial z} = 0 \quad \text{on} \quad \Sigma_H, \\ \varphi_i = 0 \quad \text{on} \quad \Sigma_-, \\ \frac{\partial \varphi_i}{\partial \mathbf{n}} = 0 \quad \text{on} \quad \Sigma_+, \end{aligned} \tag{42}$$

and φ_g is a solution to the problem

$$\begin{aligned} \frac{\partial \varphi_g}{\partial t} + L\varphi_g = 0, \\ \varphi_g = \varphi_0 \quad \text{at} \quad t = 0, \\ \frac{\partial \varphi_g}{\partial z} = \alpha \varphi_g \quad \text{on} \quad \Sigma_0, \\ \frac{\partial \varphi_g}{\partial z} = 0 \quad \text{on} \quad \Sigma_H, \\ \varphi_g = \varphi_s \quad \text{on} \quad \Sigma_-, \\ \frac{\partial \varphi_g}{\partial \mathbf{n}} = 0 \quad \text{on} \quad \Sigma_+. \end{aligned} \tag{43}$$

If we assume that all the problems (42) and (43) are solved, then we can calculate the pollution level functional for every sensitive area by

$$\begin{aligned} J_k &= \int_0^T dt \int_G p_k \varphi dG = \int_0^T dt \int_G p_k \Big(\sum_{i=1}^n Q_i \varphi_i(\mathbf{r}, t) + \varphi_g \Big) \\ &= \sum_{i=1}^n a_{ik} Q_i + b_k, \end{aligned} \tag{44}$$

where

$$a_{ik} = \int_0^T dt \int_G p_k \varphi_i dG, \tag{45}$$

$$b_k = \int_0^T dt \int_G p_k \varphi_g dG. \tag{46}$$

Now the optimization problem (39) has the form

$$
\begin{aligned}
I = \sum_{i=1}^{n} \xi_i(\bar{Q}_i - Q_i) \to \min, \\
\sum_{i=1}^{n} a_{ik} Q_i + b_k \le c_k, \quad k = 1, \dots, m.
\end{aligned}
\tag{47}
$$

Passing from Q_i to $q_i = \bar{Q}_i - Q_i$ we obtain a linear programming problem

$$
\begin{aligned}
\sum_{i=1}^{n} \xi_i q_i \to \min, \\
\sum_{i=1}^{n} a_{ik} q_i \ge R_k, \quad k = 1, 2, \dots, m, \\
q_i \ge 0, \quad i = 1, 2, \dots, n,
\end{aligned}
\tag{48}
$$

where

$$
R_k = \sum_{i=1}^{n} a_{ik} \bar{Q}_i + b_k - c_k.
$$

Thus, we have to solve in the first approach $n+1$ main problems and one linear programming problem.

ii) Adjoint equation approach. Represent the solution of the main problem (40) as the sum

$$
\varphi = \varphi_h + \varphi_g,
$$

where φ_g, as above, denotes the solution of the problem (43) and φ_h is the solution of the problem

$$
\begin{aligned}
\frac{\partial \varphi_h}{\partial t} + L\varphi_h = \sum_{i=1}^{n} \delta(\mathbf{r} - \mathbf{r_i}), \\
\varphi_h = 0 \quad \text{at} \quad t = 0, \\
\frac{\partial \varphi_h}{\partial z} = \alpha \varphi_h \quad \text{on} \quad \Sigma_0, \\
\frac{\partial \varphi_h}{\partial z} = 0 \quad \text{on} \quad \Sigma_H, \\
\varphi_h = 0 \quad \text{on} \quad \Sigma_-, \\
\frac{\partial \varphi_h}{\partial \mathbf{n}} = 0 \quad \text{on} \quad \Sigma_+.
\end{aligned}
\tag{49}
$$

Let φ_{hk}^* be the solution of the adjoint problem

$$\begin{aligned} -\frac{\partial \varphi_{hk}^*}{\partial t} - \operatorname{div}(\mathbf{u}\varphi_{hk}^*) - \mu\Delta\varphi_{hk}^* - \frac{\partial}{\partial z}(\nu\frac{\partial \varphi_{hk}^*}{\partial z}) + \sigma\varphi_{hk}^* = p_k, \\ \varphi_{hk}^* = 0 \quad \text{at} \quad t = T, \\ \frac{\partial \varphi_{hk}^*}{\partial z} = \alpha\varphi_{hk}^* \quad \text{on} \quad \Sigma_0, \\ \frac{\partial \varphi_{hk}^*}{\partial z} = 0 \quad \text{on} \quad \Sigma_H, \\ \varphi_{hk}^* = 0 \quad \text{on} \quad \Sigma_-, \\ \mu\frac{\partial \varphi_{hk}^*}{\partial n} + u_n\varphi_{hk}^* = 0 \quad \text{on} \quad \Sigma_+. \end{aligned} \tag{50}$$

Then we have the duality relation

$$\begin{aligned} \int_0^T dt \int_G p_k\varphi_h dG = \int_0^T dt \int_G \sum_{i=1}^n Q_i\delta(\mathbf{r} - \mathbf{r_i})\varphi_{hk}^* dG \\ = \sum_{i=1}^n Q_i \int_0^T \varphi_{hk}^*(\mathbf{r_i}, t)dt = \sum_{i=1}^n a_{ik}^* Q_i, \end{aligned} \tag{51}$$

where we abbreviate

$$a_{ik}^* = \int_0^T \varphi_{hk}^*(\mathbf{r_i}, t)dt. \tag{52}$$

Therefore, the pollution level functional for the sensitive area Σ_k may be calculated as follows

$$\begin{aligned} J_k = \int_0^T dt \int_G p_k\varphi dG = \int_0^T dt \int_G p_k\varphi_h dG + \int_0^T dt \int_G p_k\varphi_g dG \\ = \sum_{i=1}^n a_{ik}^* Q_i + b_k, \end{aligned}$$

where b_k is computed by (46).

Hence, the optimization problem (39) becomes

$$\begin{aligned} \sum_{i=1}^n \xi_i(\bar{Q}_i - Q_i) \to \min, \\ \sum_{i=1}^n a_{ik}^* Q_i + b_k^* \leq c_k, \quad k = 1, 2, \ldots, m, \end{aligned} \tag{53}$$

where a_{ik}^* are given by (52) and $b_k^* = b_k$.

Let us note that

$$\begin{aligned} a^*_{ik} &= \int_0^T \varphi^*_{hk}(\mathbf{r_i}, t)dt = \int_0^T dt \int_G \delta(\mathbf{r} - \mathbf{r_i})\varphi^*_{hk} dG \\ &= \int_0^T dt \int_G p_k \varphi_i dG = a_{ik}. \end{aligned}$$

As in the main equation approach, we transform the problem (53) by letting $q_i = \bar{Q}_i - Q_i$ to the form

$$\begin{aligned} &\sum_{i=1}^n \xi_i q_i \to \min, \\ &\sum_{i=1}^n a^*_{ik} q_i \geq R^*_k, \quad k = 1, 2, \ldots, m, \\ &q_i \geq 0, \quad i = 1, 2, \ldots, n, \end{aligned} \tag{54}$$

where

$$R^*_k = \sum_{i=1}^n a^*_{ik} \bar{Q}_i + b^*_k - c_k.$$

This is again a linear programming problem.

It should be noticed that in the adjoint approach before solving the linear programming problem it is necessary to solve m adjoint problems (50) and one main problem (42) while in the main equation approach we have to solve $n+1$ main problems. Thus, the choice of a method depends on the relation of m and n, namely, if $m > n$ it is better to use the adjoint approach, otherwise to use the main equation approach.

We remark that here the problem of optimization of emissions of operating plants is considered in 3D case. The 2D case was studied by Tran G.L. and Pham T.N. [19], where they carried out many experiments with the use of an up–wind difference scheme for main and adjoint problems in order to verify qualitative properties of the problem. Below we report some numerical results of the problem under consideration for two examples.

Numerical Example 1. Consider the optimization problem of emissions of plants with the following data:

- domain $G = [0, 1000] \times [0, 1000] \times [0, 50]$ (in meters)
- step sizes $dx = 20$m, $dy = 20$m, $dz = 5$m
- time of simulation $T = 4000$ sec, time step $dt = 4$ sec
- velocity vector $\mathbf{u} = (1, 0, 0)$, falling velocity $w_g = 0.1$
- diffusion coefficients $\mu = 2, \nu = 0.2$
- coefficient of transformation $\sigma = 0.005$
- 3 sensitive areas marked by rectangles:

  $\Sigma_1 = [24.5, 26.5]dx \times [25.5, 26.5]dy$ with $c_1 = 10$,
  $\Sigma_2 = [39.5, 40.5]dx \times [33.5, 35.5]dy$ with $c_2 = 30$,
  $\Sigma_3 = [39.5, 40.5]dx \times [14.5, 16.5]dy$ with $c_3 = 20$

- initial and boundary conditions are homogeneous.

- 4 sources of emissions marked by circles: the first source at point $(200, 500, 20)$ with rate 100, the second source at point $(300, 700, 30)$ with rate 70, the third source at point $(300, 300, 25)$ with rate 50 and the fourth source at point $(600, 500, 15)$ with rate 90.

- costs for reducing one unit of emission rate of plants are 1.2, 1.4, 1.0 and 1.5, resp.

The result of the numerical computation is given in the Table 1.

Source	Planned emission rate	Cost for reducing emission rates
1	88.326	14.009
2	60.670	13.062
3	36.259	13.741
4	90	0

Table 1: Optimal emission rates in Example 1.

The pollution level functionals of the sensitive areas before and after reducing emission rates are $(11.322, 34.613, 27.579)$ and $(10, 30, 20)$, respectively.

Next, the following Figures 16 and 17 show the average (in time) concentration distribution of aerosols at $z = 0$m before and after optimizing emission rates of sources, respectively.

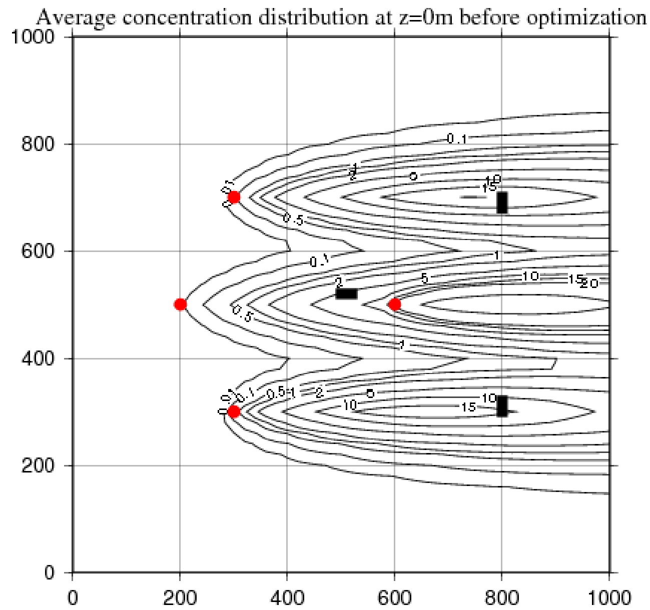

Figure 16: Average concentration distribution at $z = 0$m before optimizing sources in Example 1.

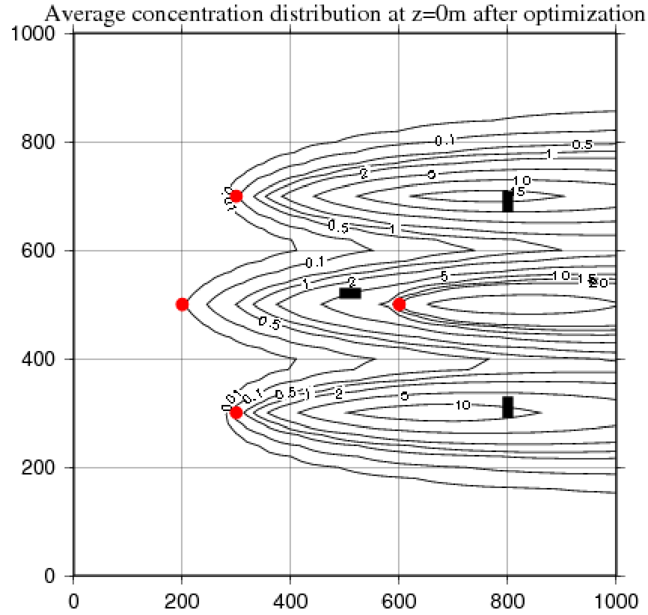

Figure 17: Average concentration distribution at $z = 0$m after optimizing sources in Example 1.

Numerical Example 2. The data in this example are the same as in the previous example except for the following changes:

- velocity vector $\mathbf{u} = (1, -0.5, 0)$
- approved pollution standards are $c_1 = 1, c_2 = 2, c_3 = 15$.

The result of calculations is given in the following Table 2.

Source	Planned emission rate	Cost for reducing emission rates
1	84.288	18.927
2	63.055	9.723
3	50	0
4	90	0

Table 2: Optimal emission rates in Example 2.

Here, the pollution level functionals of the sensitive areas before and after reducing emission rates are $(1.120, 2.061, 17.388)$ and $(1, 1.856, 15)$, respectively.

The following Figures 18–19 present the average (in time) concentration distribution of aerosols at $z = 0$m before and after optimizing emission rates of sources, respectively.

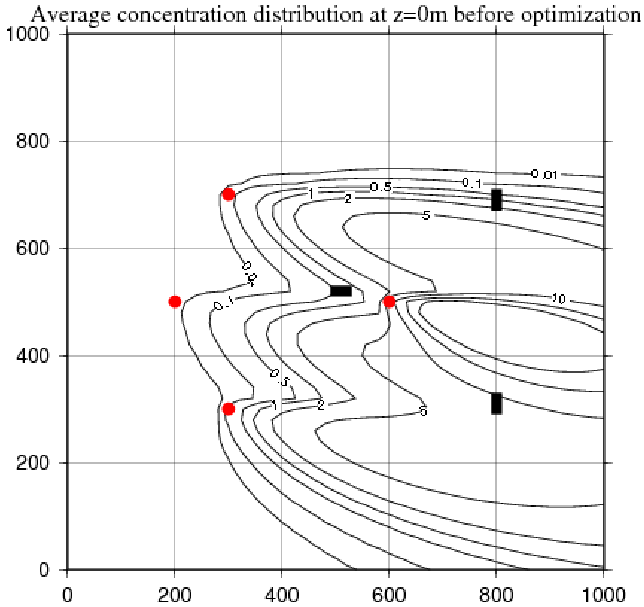

Figure 18: Average concentration distribution at $z = 0$m before optimizing sources in Example 2.

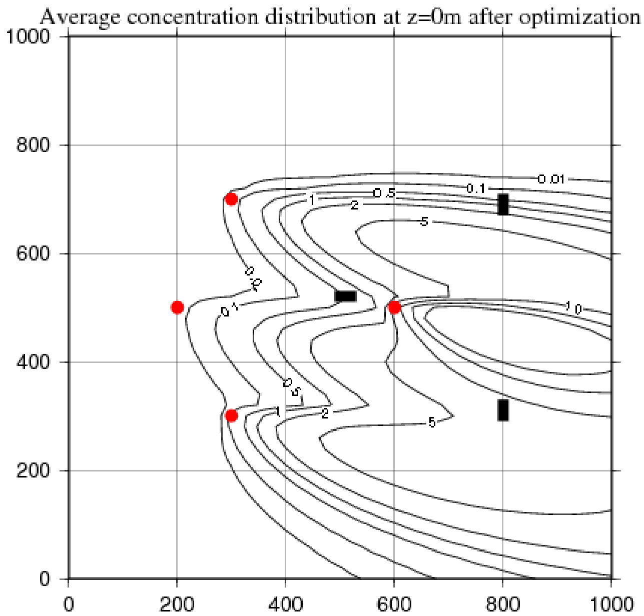

Figure 19: Average concentration distribution at $z = 0$m after optimizing sources in Example 2.

6 Determination of the coefficients of diffusion and transformation of pollutants

The coefficients of diffusion μ, ν and the coefficient of transformation σ of aerosols are important parameters of mathematical models for the study of air pollution in the atmosphere. These coefficients depend on many factors. Following Kartvelishvili [11], in general, these coefficients may depend on the concentration of aerosols. But as an approximation we suppose that they are constants and shall find them under the assumption that the concentration field of pollutants is known from measurements at grid points and at some times. Discretizing the equation (1) and considering difference equations for those grid points at those time moments where and when measurements are made, we obtain a system of equations of the form

$$\sum_{j=1}^{3} a_{ij}\lambda_j = b_i, \quad i = 1, \ldots, N,$$

where we use the notation $(\lambda_1, \lambda_2, \lambda_3) = (\mu, \nu, \sigma)$. This is a system of N equations with 3 unknowns. For finding them it is possible to use the method of least squares, which gives an approximation of μ, ν, σ with minimal error. However, this may lead to negative solution. In order to avoid this drawback, it is better to solve the following quadratic programming problem

$$\begin{gathered} \sum_{i=1}^{N}(\sum_{j=1}^{3} a_{ij}\lambda_j - b_i)^2 \to \min, \\ \lambda_i \geq 0 \quad i = 1, 2, 3. \end{gathered} \tag{55}$$

Numerical Example. For illustrating the ability of the above method we performed a numerical experiment, where the concentration field is obtained from the solution of the problem (1), (2) with the following data:

- domain $G = [0, 1000] \times [0, 1000] \times [0, 50]$ (in meters)
- step sizes $dx = 20$m, $dy = 20$m, $dz = 5$m.
- time step $dt = 4$sec
- velocity vector $\mathbf{u} = (0, 0, 0)$
- falling velocity $w_g = 0$
- diffusion coefficients $\mu = 2, \nu = 0.2$
- coefficient of transformation $\sigma = 0.005$
- source of emission $Q = 10$ at position $(100, 100, 25)$
- initial and boundary conditions are homogeneous.

We use the data of the concentration field obtained in the grid points
$(x_i, y_j, z_k),\ i = istart, ..., iend;\ j = jstart, ..., jend;\ k = kstart, ..., kend$
at times $t_m,\ \ m = mstart, ..., mend$, which for brevity we write as $(istart : iend, jstart : jend, kstart : kend, mstart : mend)$.

Below we present in Table 3 the results of computing numerically (μ, ν, σ) for various grids.

Grid domain	(μ, ν, σ) found
(0:8, 0:8, 2:6, 99:101)	(1.959, 0.205, 4.643e-4)
(0:8, 0:8, 2:6, 499:501)	(1.957, 0.205, 4.849e-4)
(0:8, 0:8, 2:6, 999:1001)	(1.957, 0.205, 4.858e-4)
(6:14, 6:14, 0:4, 99:101)	(2.021, 0.197, 6.214e-4)
(6:14, 6:14, 0:4, 499:501)	(2.072, 0.206, 5.376e-4)
(1:49, 1:49, 0:4, 499:501)	(2.012, 0.204, 4.976e-4)

Table 3: Computed values of (μ, ν, σ) for input data in various grid domains

Conclusion

In this chapter we have presented a monotone difference scheme for solving the 3D problem of diffusion and transport of aerosols in a bounded domain which ensures high accuracy and especially ensures the positivity of the solution. The realization of the scheme is reduced to solving 1D problems that require economical computational amount. Using the solution of the main problems of propagation of aerosols and their adjoint problems we solve the problem of locating new plants and the problem of optimization of emissions rates of operating industrial plants in order to keep the pollution level in given sensitive areas under a prescribed level. They are very important problems to be solved to achieve sustainable development, especially in developing countries, such as Vietnam, when foreign investment increases from year to year. A simple way for determining several parameters of the air pollution model also is proposed and experimentally studied for its applicability.

Future work will be concerned with problems in unbounded 2D and 3D domains, in domains with complicated geometry, the propagation of active aerosols and problems with complex environmental standards.

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