Atmospheric dispersion modelling in ecological engineering problems

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Abstract. The applied problems of hydrodynamics, heat and mass transfer often claim the use of numerical solution techniques in curvilinear coordinates. Such an approach is quite natural and common for flows modelling, particularly in atmosphere dynamics. The paper deals with development of atmospheric dispersion model and numerical algorithm using approximations in curvilinear coordinate systems. The approach allowed significantly simplifying the formulas and reducing the amount of computations during experiments on forecasting the air pollutants concentration nearby existing industrial plants.

1. Introduction

As is well known, the atmospheric distribution of anthropogenic and natural emissions occurs due to their advective transport by air mass and turbulent diffusion. The averaged flow of substances carried by air masses has horizontal and vertical components, and averaged fluctuation motions against a background of the main flow can be interpreted as diffusion. In addition to transport and diffusion, various internal and external perturbations are also to be taken into account in order to properly model the atmospheric dispersion process. Thus, researchers may have to deal with the complex multidimensional convection(advection)-diffusion equations together with a set of boundary conditions.

Currently, in modelling the environmental processes, there are widely used the atmospheric dispersion models developed by such eminent scientists as M.L. Barad, P.J. Barry, J.W. Deardorff, F. Gifford, G.A. Briggs, A.S. Monin, A.M. Obukhov, G.P. Marchuk, M.E. Berlyand, A.E. Aloyan, V.V. Penenko and many others. These models have been more than once thoroughly tested in practice and have proven themselves in solving a wide range of applied problems [1].

However, the further development of this scientific direction emerges new challenges and even problem areas where existing models require too much resources or lead to unacceptably large error margins, and sometimes may not be applicable at all.

It should be noted that the mass transfer in a horizontal plane is usually described using the Cartesian coordinate system. In the dynamics of the atmosphere the directions by x and y axes are taken as east and north, respectively.
Meanwhile, many applied problems of hydrodynamics, heat and mass transfer, which researchers are faced with, require the use of curvilinear grids for numerical solution [2]. Therefore, it becomes appropriate to obtain formulas for the coefficients of a discrete analogue of differential equations using approximations in curvilinear coordinate systems like cylindrical or spherical coordinates. Such a choice of system parameters is natural and very common when modelling flows in mathematical physics [3], for example, when modelling the atmosphere or ocean dynamics [4, 5].

Specifically with regard to modelling of air pollution dispersion, in most cases the Cartesian coordinate system meets all the needs, since the scale of motion description is not so large to necessitate taking into account the curvature of the Earth's surface. Though, the use of curvilinear coordinate systems here is not limited to describing large-scale movements on the surface of the globe.

For example, if we consider the case of heavy impurity emission from point industrial source, then the air pollution concentration will largely depend on the deposition rate, which in turn depends on the density and size of the aerosol particles. In this case, the plume contours will have an arched shape in longitudinal section (figure 1).

Figure 1. Schematic representation of air pollution emission plume.

Figure 1 illustrates so-called tilted plume model [6]. Here $u$ is the wind speed in the direction of the $x$ axis; $h$ is the effective plume height; $w_g$ is the particles deposition rate. The plume axis tilts with speed $w_g$. The nature of the distribution of aerosol particles concentration in the atmospheric surface layer and deposited on the ground for similar situations was previously established experimentally. For instance, if we have $h=100 \text{ m}$, $u=5 \text{ m/sec}$, 20 $\mu$m - diameter particles with densities of 5 $\text{g/cm}^3$, then about half of the volume of aerosol emission will deposit within a distance of 8.3 km [6].

Thus, in fact, for a system of convection-diffusion equations the gridded region of solution can be considered not as parallelepiped, but as a hemisphere (figure 2).

Figure 2. The problem of region solution.
Then, the usefulness of curvilinear coordinate system will be justified by the fact that it will allow us significantly simplify the formulation of boundary conditions [5] and reduce the amount of computation.

2. Governing equations

The process of air pollution dispersion, taking into account meteorological factors and other disturbances, is described by following multidimensional partial differential equation [7, 8]:

\[
\frac{\partial \theta}{\partial t} + u \frac{\partial \theta}{\partial x} + v \frac{\partial \theta}{\partial y} + \left(w - w_g\right) \frac{\partial \theta}{\partial z} + \sigma \theta = \frac{\partial}{\partial z} \left( k \frac{\partial \theta}{\partial z} \right) + \mu \Delta \theta + Q \delta(\mathbf{r} - \mathbf{r}_0).
\]  

(1)

Here, \( \theta \) – contaminants concentration in the atmosphere; \( \theta_0 \) – initial contaminants concentration; \( x, y, z \) – coordinate system; \( \sigma \) – atmospheric absorption coefficient; \( \mu, k \) – diffusion and turbulence coefficients; \( \delta_{i,j,k} \) – Dirac function; \( Q \) – emitter capacity; \( \Delta \) – the Laplace operator.

It should be noted that the components of the vector of air mass flow velocity depend on such external parameters as temperature stratification and the Rossby number, which, in turn, require solving the equation of the heat balance of the earth’s surface. To avoid excessive complication of the differential equations, let us assume that \( u, v, w = \text{const} \) on each time interval \( [0, t_1), [t_1, t_2), [t_2, t_3), [t_3, t_4), \ldots, (t_{n-1}, t_n) \).

Also, to simplify the mathematical model and increase the order of finite difference approximation (in spatial variables), we use next relation

\[
\tilde{w} = w - w_g; \quad \theta(x, y, z, t) = e^{-2\mu + \frac{w_g}{2k \tilde{\theta}(x, y, z, t)}}
\]

and, assuming the \( k = \text{const} \), we transform equation (1) into the following form [7, 8]:

\[
\frac{\partial \tilde{\theta}(x, y, z, t)}{\partial t} + \sigma_1 \tilde{\theta}(x, y, z, t) = \mu \frac{\partial^2 \tilde{\theta}(x, y, z, t)}{\partial x^2} + \mu \frac{\partial^2 \tilde{\theta}(x, y, z, t)}{\partial y^2} + k \frac{\partial^2 \tilde{\theta}(x, y, z, t)}{\partial z^2} + e_1 \tilde{\theta}(x, y, z, t)Q,
\]

(2)

where

\[
\sigma_1 = \frac{k u^2 + k v^2 + \mu w^2 + 4\sigma_1 k \mu}{4 \mu k}; \quad e_1 = e^{-\frac{(u x + v y + w g)}{2k \tilde{\theta}(x, y, z, t)}}.
\]

First, let us consider the equation (2) in a parallelepiped \( D = \{0 \leq x \leq L_4; 0 \leq y \leq L_2; 0 \leq z \leq L_3\} \).

Then, for the problem closure, we add the following initial and boundary conditions:

\[
\tilde{\theta}(x, y, z, t)_{|t=0} = \tilde{\theta}^0(x, y, z);
\]

(3)

\[
-\mu \frac{\partial \tilde{\theta}(x, y, z, t)}{\partial x} \bigg|_{x=0} = \xi (e_1 \theta_E - \tilde{\theta}(0, y, z, t));
\]

(4)

\[
\mu \frac{\partial \tilde{\theta}(x, y, z, t)}{\partial x} \bigg|_{x=L_4} = \xi (e_1 \theta_E - \tilde{\theta}(L_4, y, z, t));
\]

(5)

\[
\mu \frac{\partial \tilde{\theta}(x, y, z, t)}{\partial x} \bigg|_{x=L_1}
\]
\[-\mu \frac{\partial \tilde{\theta}(x, y, z, t)}{\partial y}\bigg|_{y=0} = \xi \left(e_i \theta_E - \tilde{\theta}(x, 0, z, t)\right); \quad (6)\]

\[\mu \frac{\partial \tilde{\theta}(x, y, z, t)}{\partial y}\bigg|_{y=L_2} = \xi \left(e_i \theta_E - \tilde{\theta}(x, L_2, z, t)\right); \quad (7)\]

\[-\kappa \frac{\partial \tilde{\theta}(x, y, z, t)}{\partial z}\bigg|_{z=0} = \left(\beta \tilde{\theta}(x, y, 0, t) - e_i f_0(x, y)\right); \quad (8)\]

\[\kappa \frac{\partial \tilde{\theta}(x, y, z, t)}{\partial z}\bigg|_{z=L_3} = \xi \left(e_i \theta_E - \tilde{\theta}(x, y, L_3, t)\right). \quad (9)\]

The numerical solution of the problem (2) – (9) for various kinds of conditions is given in [7, 8] and it does not give rise to any special difficulties.

Now, returning to the essence of this work, let us note that when the spatial distribution of harmful emissions expands, the number of receptors in the gridded region of the problem solution increases significantly as well as the amount of computations. In order to avoid this trouble, we turn to curvilinear coordinate systems.

3. Derivation of equations for curvilinear coordinates

3.1. The right circular cylinder

In such a case the problem statement and its numerical solving method will become more simple. The problem solution region will look as \( D = \{0 < r < R, 0 < \lambda < 2 \cdot \pi, 0 < z < L\} \), and the process of atmospheric dispersion now can be described using the equation

\[
\frac{\partial \theta}{\partial t} + u \frac{\partial \theta}{\partial r} + v \frac{\partial \theta}{\partial \lambda} + w \frac{\partial \theta}{\partial z} + \sigma \cdot \theta = \mu \left(\frac{1}{r} \frac{\partial}{\partial r} \left( r \frac{\partial \theta}{\partial r} \right) + \frac{1}{r^2} \frac{\partial^2 \theta}{\partial \lambda^2}\right) + k \frac{\partial^2 \theta}{\partial z^2} + Q \delta(r - R_0) \quad (10)
\]

with boundary conditions

\[
\theta(r, \lambda, z, 0) = \theta(r, \lambda, z); \quad (11)
\]

\[
\left\{
\begin{aligned}
-\alpha_{11} r \frac{\partial \theta}{\partial r} - \beta_{11} \cdot \theta &= \mu_{11} \quad \text{for } r = R; \\
\alpha_{21} \cdot k \frac{\partial \theta}{\partial z} - \beta_{21} \cdot \theta &= -\mu_{21} \quad \text{for } z = 0; \\
-\alpha_{22} \cdot k \frac{\partial \theta}{\partial z} - \beta_{22} \cdot \theta &= -\mu_{22} \quad \text{for } z = l;
\end{aligned}
\right. \quad (12)
\]

Here again, may be conditions of the first, second and third kind or mixed type, depending on the parameters’ values. For \( \alpha_{m,n} = 0 \) we obtain the first boundary value problem, for \( \beta_{m,n} = 0 \) – the second boundary value problem, and for \( \alpha_{m,n} \neq 0 \) and \( \beta_{m,n} \neq 0 \) – the third boundary value problem.
(m = 1, 2, 3; n = 1, 2). If $\alpha_{m,n}$ and $\beta_{m,n}$ do not simultaneously vanish, then at the edges of the region we obtain conditions of various kinds.

Problem (10) - (12) can be solved by a similar difference method as that in [7, 8].

3.2. The sphere

The equation (1) can be considered in the region $D = \{0 < r < h, 0 \leq \lambda \leq 2 \cdot \pi, 0 < \eta < \pi\}$, which is a sphere with radius $R$. Then equation (1) takes the form

$$\frac{\partial \theta}{\partial t} + \sigma \cdot \theta = \frac{1}{r^2} \frac{\partial}{\partial r} \left( r^2 k \frac{\partial \theta}{\partial r} \right) + \left( \frac{1}{r^2 \sin \theta} \frac{\partial}{\partial \eta} \sin \eta \frac{\partial \theta}{\partial \eta} + \frac{1}{r^2 \sin^2 \eta} \frac{\partial^2 \theta}{\partial \lambda^2} \right) + Q \delta(r - r_0), \quad (13)$$

and the boundary conditions are written as

$$\theta(r, \lambda, \eta, 0) = \theta(r, \lambda, \eta) \quad \text{for} \quad t = 0; \quad (14)$$
$$-\alpha_r r^2 k \frac{\partial \theta}{\partial r} - \beta_1 \cdot \theta = -\mu_1 \quad \text{for} \quad r = R_1; \quad (15)$$
$$\theta(r, \lambda, \eta, t) = \theta(r, \lambda + 2 \cdot \pi, \eta, t).$$

Here, such conditions with respect to $r$ can be of the first, second and third kind.

3.3. The hemisphere

If the equation (1) is considered in the hemisphere, then for $\eta = \frac{\pi}{2}$ we set the condition

$$-\alpha_2 \sin \eta \frac{\partial \theta}{\partial \eta} - \beta_2 \cdot \theta = -\mu_2,$$

and if the solution region is

$$D = \{R_1 < r < R_2, \lambda_1 < \lambda < \lambda_2, \eta_1 < \eta < \eta_2, R_1 < R_2, \lambda_2 - \lambda_1 < 2 \cdot \pi, \eta_2 - \eta_1 < \pi\},$$

then the boundary conditions are written as

$$\alpha_{1,1} r^2 k \frac{\partial \theta}{\partial r} - \beta_{1,1} \cdot \theta = -\mu_{1,1} \quad \text{for} \quad r = R_1; \quad (16)$$
$$-\alpha_{1,2} r^2 k \frac{\partial \theta}{\partial r} - \beta_{1,2} \cdot \theta = -\mu_{1,2} \quad \text{for} \quad r = R_2;$$
$$\alpha_{2,1} \sin \eta \frac{\partial \theta}{\partial \eta} - \beta_{2,1} \cdot \theta = -\mu_{2,1} \quad \text{for} \quad \eta = \eta_1;$$
$$-\alpha_{2,2} \sin \eta \frac{\partial \theta}{\partial \eta} - \beta_{2,2} \cdot \theta = -\mu_{2,2} \quad \text{for} \quad \eta = \eta_2.$$

In this case, there may also be conditions of the 1st, 2nd and 3rd kind, and the solution algorithm posed no difficulty.

4. Numerical algorithm

The problem (10) - (12) is solved by the difference method as that in [9]. First, we generate a grid in $t$

$$\omega_t = \{t_n = n \Delta t, n = 1, 2, \ldots\}.$$
and then we write the equation (10) at the time \( t = t_n \)

\[
\frac{\theta^{n+1} - \theta^n}{\Delta t} + \delta \theta^n + 1 = L_z \theta^{n+1} + L_r \theta^{n+1} + L_\lambda \theta^{n+1} + f^{n+1},
\]

(17)

where

\[
L_z = \frac{\partial}{\partial z} + \frac{\partial}{\partial \zeta}, \quad L_r = \mu \frac{\partial}{\partial r} + \frac{\partial}{\partial \zeta} r, \quad L_\lambda = \mu \frac{\partial^2}{\partial \lambda^2} + f^{n+1} = Q(\vec{r} - \vec{r}_0).
\]

Eventually, instead of the equation (17) we obtain the Helmholtz equation

\[
(L_z + L_r + L_\lambda) \phi^{n+1} - \left( \frac{1}{\Delta t} + \delta \right) \phi^n = -f^{n+1}(z, r, \lambda),
\]

(18)

where

\[
\tilde{f}^{n+1}(z, r, \lambda, t_{n+1}) = f^{n+1} + \frac{1}{\Delta t} \phi^n.
\]

Thus, the solution of the equation (10) was reduced to the three-dimensional Helmholtz equation which is solved at each time step. And to do that, we multiply the equation (18) on both sides by \( r^2 \), then we replace the differential operator in \( t \) by the difference operator and get the following

\[
(L_r + L_\zeta + L_\lambda) \theta^{m+1} - r^2 \left( \frac{1}{\Delta t} + \delta \right) \theta^n = -f^{n+1},
\]

(19)

where

\[
L_r = \frac{\partial^2}{\partial r^2} + r \frac{\partial}{\partial r}, \quad L_\zeta = \frac{\mu}{\sin \zeta} \frac{\partial}{\partial \zeta} \sin \zeta \frac{\partial}{\partial \zeta}, \quad L_\lambda = \frac{\mu}{\sin^2 \zeta} \frac{\partial^2}{\partial \lambda^2}; \quad f^{n+1} = r^2 \theta(\vec{r} - \vec{r}_0) + \frac{1}{\Delta t} \theta^n r^2
\]

Further, we add the following boundary conditions to the equation (10)

\[
-\alpha_r \frac{\partial \theta^{n+1}}{\partial r} - \beta_r \theta^{n+1} = -\mu_t^{n+1}, \quad r = R; \quad \theta^{n+1}(r, \lambda, \zeta, t) = \theta^{n+1}(r, \lambda + 2\pi, \zeta, t).
\]

Equation (19) is a three-dimensional equation of elliptic type with separable variables. Hereinafter, in order to avoid the complication of the equation writing, we omit the superscript.

Let us generate the grid

\[
\omega_r = \{ r_i = (i + 0,5) h_r, \quad i = 0,1,\ldots, N + 1, \quad h_r = R / (N_r + 1,5) \},
\]

and write the equation (19) for \( r = r_i \) taking into account the boundary conditions, that gives us a system of equations

\[
(L_\zeta - L_\lambda) \Phi + A_r \Phi = -F,
\]

(20)

where

\[
F = \left[ f_0, f_1, \ldots, f_{N_t+1} + \frac{2 \mu_t}{h_r a_t} \right]; \quad A_r = \begin{pmatrix}
-h_0 & c_0 & 0 & \cdots & 0 & 0 \\
0 & a_1 & -b_1 & c_1 & 0 & \cdots \\
0 & 0 & a_2 & \cdots & \cdots & \cdots \\
0 & 0 & \cdots & a_{N_t+1} & -b_{N_t+1}
\end{pmatrix}.
\]
\[ c_0 = \frac{2}{r_0 h_r^2}; \quad b_0 = c_0 + r_1 \left( \frac{1}{\Delta t} + \delta \right); \quad a_i = -r_i^2 \frac{1}{h_r^2}; \quad c_i = -r_i^2 \frac{1}{h_r^2}; \quad b_i = a_i + c_i + \left( \frac{1}{\Delta t} + \delta \right) r_i^2, \quad i = 1, 2, \ldots, N_i; \]

\[ a_{N_i+1} = -\frac{2 r_i^2}{h_r^2}; \quad b_{N_i+1} = a_{N_i+1} + \frac{2 \beta_i}{h_i^2} + \left( \frac{1}{\Delta t} + \delta \right) r_i^2 \frac{3}{4}. \]

The matrix \( A_r \) can be represented as \( A_r = B_r \Lambda_r B_r^{-1} \), where the columns of the matrix \( B_r \) are the eigenvectors of \( A_r \) corresponding to the eigenvalue \( \lambda_i \) of \( A_r \). \( \Lambda_r = \left[ \lambda_0, \lambda_1, \ldots, \lambda_{N_i} \right] \) is the diagonal matrix consisting of the eigenvalues of the matrix \( A_r \).

Multiplying (20) by \( B_r^{-1} \), we obtain the transformed equation

\[ (L_{0\theta} + L_{\lambda}) \theta_i^{(1)} - \gamma_i^{2} \theta_i^{(1)} = -f_i^{(1)}, \quad (21) \]

where

\[ B_r^{-1} \Phi = \Phi^{(1)} = \left( \theta_0^{(1)}, \theta_1^{(1)}, \ldots, \theta_{N_i}^{(1)} \right); \quad \gamma_i^{2} = -\lambda_i, \quad i = 0, 1, 2, \ldots, N_i + 1. \]

Accordingly, the periodicity condition is also transformed to

\[ \theta_i^{(1)}(\theta, \lambda) = \theta_i^{(1)}(\theta, \lambda + 2\pi). \]

Now, we introduce the grid in \( \lambda \):

\[ \omega_\lambda = \left\{ \lambda_j = j \cdot h_\lambda, \quad j = 1, 2, \ldots, N_2 \right\}. \]

Then, we replace the differential operator in \( \lambda \) by the difference one, and transforming it, we obtain the following differential equation

\[ \mu \frac{1}{\sin \xi} \frac{\partial}{\partial \xi} \sin \xi \frac{\partial \theta_{i,j}^{(2)}}{\partial \xi} - \left( \gamma_{i,1}^{2} + \gamma_{i,2}^{2} \frac{1}{\sin^{2} \xi} \right) \theta_{i,j}^{(2)} = -f_{i,j}^{(2)}, \quad (22) \]

where

\[ P_{i,j}^{*} \Phi_{i}^{(1)} = \Phi_{i}^{(2)} = \left( \theta_{i,j}^{2}, \theta_{i,j+1}^{2}, \ldots, \theta_{i,N_2}^{2} \right); \]

\[ P_{i,j}^{*} F_{i}^{(1)} = F_{i}^{(2)} = \left( f_{i,j+1}^{2}, f_{i,j+2}^{2}, \ldots, f_{i,N_2}^{2} \right); \]

\[ \gamma_{i,j}^{2} = -\left( 2 - \lambda_{i,j} \cdot \frac{\mu}{h_\xi^2} \right), \quad i = 0, 1, \ldots, N_1 + 1, \quad j = 1, 2, \ldots, N_2. \]

Next, in the equation (22) we replace the differential operator with the difference one, and obtain a three-point system of equations with diagonal dominance, which is solved by the matrix sweep algorithm. Knowing \( \theta_{i,j,k}^{(2)} \), with the help of (21), (23), from the function \( \theta_{i,j,k}^{(2)} \) we turn to the function

\[ \theta_{i,j,k} = \sum_{s_i=0}^{N_1+1} \sum_{s_2=0}^{N_2} b_{i,s_i,s_1} \cdot P_{i,s_2}^{*} \theta_{s_2,s_2,k}^{(2)}, \]
Finally, repeating this process $n$ times, we obtain the problem solution at time $t_n = n\Delta t$.

5. Conclusions
In the light of the foregoing, we can conclude that we have derived the mathematical models of the process of atmospheric dispersion process using approximations in curvilinear coordinate systems. In order to solve the systems of convection-diffusion equations, there was developed conservative numerical algorithm.

The considered approach allowed us significantly simplify the formulas and reduce the amount of computations during experiments on forecasting the air pollutants concentration in the vicinity of working industrial sites in Samarkand and Tashkent regions.

The developed mathematical software can be applied in settling various ecological engineering problems such as optimal allocation of newly projected industrial sites, evaluation of the spread of industrial contamination over adjacent territories and forecast the negative impact on the environment as well as in support of decision-making on possible ecological risks minimization.

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