RECONSTRUCTION OF AIR POLLUTION FIELD IN GEOGRAPHIC REGIONS BASED ON A POLLUTION TRANSFER MODEL

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A technique is proposed for reconstructing the field of air pollution averaged vertically over the height of the atmospheric planetary boundary layer, horizontally over the area of a grid cell, and temporally. The technique is based on the numerical solution of the pollutant transfer equation with the help of the matrix theory and employs the data on emissions of pollutants as well as the climatic data on wind velocity and precipitation. The technique has been implemented at the m×n grid nodes (m, n = 12), and the results of reconstructing the sulphurous gas concentration in January and July over Eastern States of the U.S.A and adjoining area of the Atlantic Ocean have been presented.

INTRODUCTION

Air, soil, and water pollution by the waste products of industrial, agricultural, and other anthropogenic origin has a strong adverse effect on the ecology of individual districts and large geographical regions.

Because of this, increasingly much attention is devoted to environmental monitoring through the development of an integrated system of observations and theoretical estimates of environmental state.[2,4,13,14,16]

In Russia, this purpose is met through the special Program on Ecological Safety of Russia. As a result of its implementation, Russia will be divided into regions according to the degree of ecological hazard.[5] When done on a global scale, such study makes it possible to reveal the statistical models of ecologically homogeneous regions, as was done in Ref. 9, for example, for temperature and some gaseous components of the atmosphere. Noteworthy, this study can be accomplished successfully using geoinformational approaches.[10]

Still considered as highly promising are the methods of estimating the ecological situation, particularly of air pollution level, based on the physico–mathematical models of pollutant transfer implemented on a computer.[4,6,11,15,17,18] However, an estimate of the level of air pollution in the regions (such as oceanic and polar) in which the pollutant concentration does not measured at all, presents serious problem.

The present paper proposes a method for reconstructing time– and space–average air pollution field over such regions with the availability of climatic data. The method employs numerical solution[3] of the pollutant transfer equation as well as the matrix theory.[7,8,12]

TECHNIQUE FOR RECONSTRUCTING THE AIR POLLUTION FIELD

The technique is based on the equation of transfer of arbitrary pollutant

$$\frac{\partial s}{\partial t} + u\frac{\partial s}{\partial x} + v\frac{\partial s}{\partial y} + w\frac{\partial s}{\partial z} + \frac{\partial w_a s}{\partial z} = k_1 \Delta s + \frac{\partial}{\partial z} k \frac{\partial s}{\partial z} + \varepsilon_a , \quad (1)$$

where s is the volume concentration of the pollutant, ε_a is the rate of generation or removal of the pollutant a in unit air volume, $k = k(z)$ and k_1 are the vertical and horizontal turbulent exchange coefficients, w_a is the intrinsic vertical velocity of the pollutant a, and

$$\Delta = \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} .$$

For the purpose of reconstructing the concentration of pollutant in the planetary boundary layer (PBL) of height H (Ref. 3), we impose the following boundary conditions:

$$z = H: \ w = w_a = 0 , \ \ k = k_1 = 0 ,$$

$$z = 0: \ k\frac{\partial s}{\partial z} - w_a s_0 = \beta s_0 - f_0 , \quad (2)$$

where s_0 is the s value at $z = 0$, β is the rate of "dry" absorption of the pollutant by the Earth's surface, and $f_0 = f_0(x, y)$ is the upward flow of the pollutant from the ground.

The function ε_a is given by expression

$$\varepsilon_a = F - W - R , \quad (3)$$

where F is the emission rate of pollution sources, $W = \sigma_2 s$ is the rate of "wet" removal of the pollutant (its washing out by precipitation), $R = \sigma_3 s$ is the rate of the chemical transformation of the given pollutant into the other, and σ_2 and σ_3 are the coefficients.

To solve Eq. (1) by numerical techniques in a grid cell,[3] we first integrate it vertically from $z = 0$ to $z = H$, horizontally from $x = -\delta/2$ to $x = \delta/2$ and from $y = -\delta/2$ to $y = \delta/2$, with $\delta = \Delta x = \Delta y$ being the grid step, as well as temporally from $t = t_1$ to $t = t_2$, with time interval $t_1 - t_2$ chosen arbitrary as day, month, year, etc. We introduce averaging over space and time by the following relations:

$$\overline{s} = \frac{1}{(t_2 - t_1)\,\delta^2 H} \int_{t_1}^{t_2} \int\int_{-\delta/2}^{\delta/2} \int_0^H s(x, y, z, t)\, dz\, dx\, dy\, dt ,$$

$$\overline{u} = \frac{1}{(t_2 - t_1)\,\delta^2 H} \int_{t_1}^{t_2} \int\int_{-\delta/2}^{\delta/2} \int_0^H u(x, y, z, t)\, ds\, dx\, dy\, dt , \quad (4)$$

etc.

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Integration of Eq. (1) with boundary condition given by Eq. (2) on account of Eq. (4), dropping insignificant terms, yields the following equation for averages:

$$\frac{\partial \bar{s}}{\partial t} + u\frac{\partial \bar{s}}{\partial x} + v\frac{\partial \bar{s}}{\partial y} = -\bar{\sigma}\,\bar{s} + k_1 \Delta \bar{s} + \bar{\varphi}\ , \quad (5)$$

where

$$\bar{\varphi} = \bar{F} + \frac{1}{H}\bar{f}_0\ . \quad (6)$$

We note that in the derivation of Eq. (5) we express s_0 in terms of $\bar{s}$ as $s_0 = \alpha_0 \bar{s}$, with $\alpha_0 = s_0/\bar{s}$ being an empirical constant.

When averaging over extended periods of the order of month, the derivative $\partial s/\partial t$ is negligible in comparison with the other terms. Then the above equation reduces to

$$u\frac{\partial s}{\partial x} + v\frac{\partial s}{\partial y} = -\sigma s + k_1 \Delta s + \varphi \quad (7)$$

(the bar atop is omitted).

This yields the stationary boundary–value problem that can be solved for average values disregarding the vertical motion and the turbulence at the PBL top. As to the chemical transformation (R) of a given pollutant, it can be accounted for in general by assuming a portion of the incoming pollutant to be transformed into the other constituents just after entering the atmosphere. This way, $(1-\gamma)F$ and $(1-\gamma)f_0$ are used in place of F and f_0, with γ being the transforming portion of the examined pollutant ($\gamma \approx 0.1$). Accordingly, the variable σ in Eq. (7) can be represented as

$$\sigma = \sigma_1 + \sigma_2\ ,$$

where $\sigma_1 = (\beta/H)\,\alpha_0$ and $\sigma_2 = \alpha^* I$ (I is the precipitation intensity, α^* is a coefficient). The ratio $\beta/H = k_{\mathrm{abs}}$ can be interpreted as the coefficient of "dry" absorption of the pollutant by the surface, while $\sigma_2 = k_{\mathrm{wash}}$ as the coefficient of its washing out by precipitation.[11]

MATHEMATICAL IMPLEMENTATION OF THE MODEL

We now replace differential equation (7) of the stationary boundary–value problem with its corresponding finite–difference analog.[3,7] For this, let us introduce a grid of points (see Fig. 1) and a new coordinate system $j = x/\delta$ and $i = -y/\delta$, where $\delta = \Delta x = \Delta y$. We note that introducing this notation, in the subsequent matrix analysis i and j will denote columns and rows of the rectangular matrix A_{ij}. The derivatives with respect to x and y in terms of the centered difference become[3,7]

$$\left(\frac{\partial s}{\partial x}\right)_{ij} = \frac{1}{2\delta}(s_{i,j+1} - s_{i,j-1}),\ \left(\frac{\partial s}{\partial y}\right)_{ij} = \frac{1}{2\delta}(s_{i-1,j} - s_{i+1,j}),$$

$$(\Delta s)_{ij} = \left(\frac{\partial^2 s}{\partial x^2}\right)_{ij} + \left(\frac{\partial^2 s}{\partial y^2}\right)_{ij} =$$

$$= \frac{1}{\delta^2}(s_{i+1,j} + s_{i-1,j} + s_{i,j+1} + s_{i,j-1} - 4\,s_{ij})\ .$$

In this case differential equation (7) transforms into its finite–difference analog

$$u_{ij}\frac{1}{2\delta}(s_{i,j+1} + s_{i,j-1}) + v_{ij}\frac{1}{2\delta}(s_{i-1,j} - s_{i+1,j}) -$$
$$-\frac{k_1}{\delta^2}(s_{i,j+1} + s_{i,j-1} + s_{i-1,j} + s_{i+1,j} - 4\,s_{ij}) - \sigma_{ij}\,s_{ij} = \varphi_{ij}\ , \quad (8)$$

which upon multiplying by δ^2/k_1 and collecting terms becomes

$$a_{ij}s_{i,j+1} + b_{ij}s_{i,j-1} + c_{ij}s_{i-1,j} + d_{ij}s_{i+1,j} + e_{ij}s_{ij} = g\,\varphi_{ij} \quad (9)$$
$$(i = 1, 2, \ldots, m\ ;\ j = 1, 2, \ldots, n).$$

In the inner calculation region, the coefficients a_{ij}, b_{ij}, etc. are expressed as

$$a_{ij} = \left(1 - \frac{\delta}{2k_1}u_{ij}\right),\quad b_{ij} = \left(1 + \frac{\delta}{2k_1}u_{ij}\right),$$

$$c_{ij} = \left(1 - \frac{\delta}{2k_1}v_{ij}\right),\quad d_{ij} = \left(1 + \frac{\delta}{2k_1}v_{ij}\right),$$

$$e_{ij} = \left(-4 + \sigma_{ij}\frac{\delta^2}{k_1}\right),\qquad g = \frac{\delta^2}{k_1}\ . \quad (10)$$

The coefficients of variables s_{ij} beyond the calculation region differ from those within it (see Fig. 1, $i = 0$, $m+1$ and $j = 0$, $n+1$) and are extrapolated from the latter by the formula

$$f(x) = f(x_0) + (\mathrm{d}f/\mathrm{d}x)_{x = x_0}\,\Delta x\ .$$

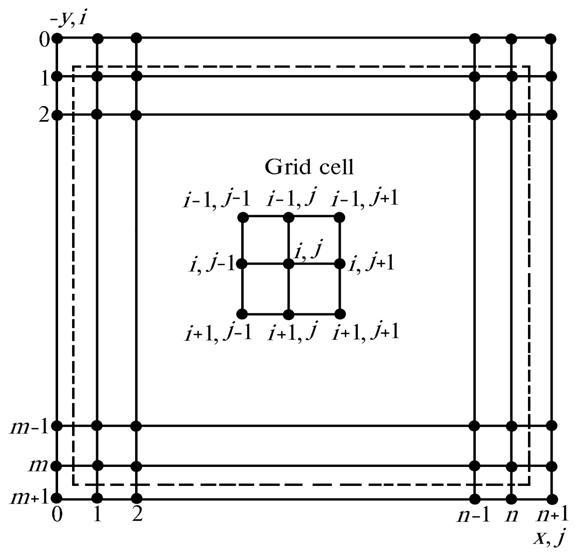

FIG. 1. Calculational grid cells. Dashed curve marks the region for calculation of m×n derivatives s_{ij}.

For left–most row (except for the corner points), with the use of this expression we derive

$$f(j=0) = f(j=1) - (2\,f(j=2) - f(j=1)\,\delta)/\delta =$$
$$= 2\,f(j=1) - f(j=2).$$

More generally, we obtain

$$f_{i,\,j=0} = q_1\,f_{i,\,j=1} - q_2\,f_{i,\,j=2}\ ,$$

where q_1 and q_2 are coefficients.

Equation (9) is a system of $m\times n$ linear algebraic equations with $m\times n$ unknowns. In matrix notation, it is written as

$$A\,x = b\ , \quad (11)$$

where A is the square matrix ($m = n$),

$$A = A_{i\,j} = \begin{bmatrix} A_{1,1} & A_{1,2} & \dots & A_{1,\,m} \\ A_{2,1} & A_{2,2} & \dots & A_{2,\,m} \\ \dots & \dots & \dots & \dots \\ A_{m,1} & A_{m,2} & \dots & A_{m,\,m} \end{bmatrix},$$

and b is the matrix of right–hand sides of the equation,

$$b = b_{i\,k} = \begin{bmatrix} b_{1,1} & b_{1,2} & \dots & b_{1,\,n} \\ b_{2,1} & b_{2,2} & \dots & b_{2,\,n} \\ \dots & \dots & \dots & \dots \\ b_{n,1} & b_{n,2} & \dots & b_{n,\,n} \end{bmatrix}.$$

The elements of matrices $A_{i\,j}$ and $b_{i\,k}$ are determined by the coefficients $a_{i\,j}$, $b_{i\,j}$, etc., from equation (10) as well as by the expression for $\varphi_{i\,j}$.

A solution to the system of equations (9) and (11) can be expressed in the form[7,12]

$$x = A^{-1}\, b\,,$$

where A^{-1} is the inverse matrix such that

$$A \times A^{-1} = E\,,$$

where E is the unit matrix of the form[7,12]

$$E = E(\delta_{i\,j}) = \begin{bmatrix} 1 & 0 & \dots & 0 \\ 0 & 1 & \dots & 0 \\ \dots & \dots & \dots & \dots \\ 0 & 0 & \dots & 1 \end{bmatrix}.$$

The inverse matrix

$$A_{i\,j}^{-1} = \begin{bmatrix} A_{1,1}^{-1} & A_{1,2}^{-1} & \dots & A_{1,\,m}^{-1} \\ A_{2,1}^{-1} & A_{2,2}^{-1} & \dots & A_{2,\,m}^{-1} \\ \dots & \dots & \dots & \dots \\ A_{m,1}^{-1} & A_{m,2}^{-1} & \dots & A_{m,\,m}^{-1} \end{bmatrix}$$

is related to the sought–after matrix $x_{ik}(s_{ik})$ as

$$x_{i\,k} = \sum A_{i\,j}^{-1}\, b_{i\,k} = A_{i,\,1}^{-1}\, b_{1,\,k} + A_{i,\,2}^{-1}\, b_{2,\,k} + \dots + A_{i,\,n}^{-1}\, b_{n,\,k}\,,$$

whose $\overline{i,j}$ th element is the sum of products of the elements of ith row of matrix A^{-1} and kth column of the matrix b.

The matrix of the sought–after unknowns can be represented in the form

$$s_{i\,k} = [\,x_{i\,j}] = \begin{bmatrix} s_{1,1} & s_{1,2} & \dots & s_{1,\,m} \\ s_{2,1} & s_{2,2} & \dots & s_{2,\,m} \\ \dots & \dots & \dots & \dots \\ s_{m,1} & s_{m,2} & \dots & s_{m,\,m} \end{bmatrix}.$$

Computionally, most difficult problem is to find the inverse matrix A^{-1}. The efficient inversion procedure was proposed by Ershov.[8] It was repeatedly employed for statistical forecast. In that case the initial matrix order was as high as 45 (min = 45).

The inversion proceeds as follows. We first replace the initial matrix by the matrix $C^{(0)} = A - E(\delta_{ij})$, and then construct two successive matrices $C^{(1)'}$, $C^{(1)}$, ... $C^{(n)'}$, $C^{(n)}$, ... , whose elements are given by the relations

$$C^{(m)'} = \frac{C_{i\,j}^{(m-1)}\ (i = m)}{\delta_{mj}\ \ (i = m)}\ (i, j = 1, \dots, n\,;\ m = 1, \dots, n);$$

$$C_{i\,j}^{(m)} = C_{i\,j}^{(m)'} - \frac{C^{(m)'}}{1 + C_{m\,m}^{(m-1)}}\, C_{m\,j}^{(m-1)}\,.$$

Matrix $C^{\,m-n}$ is just the derived inverse matrix A^{-1} of the initial matrix A.

PRACTICAL APPLICATION OF THE MODEL

The above–described technique was used to calculate the average monthly concentration of sulphurous gas in January and July over North–Eastern States of the U.S.A. and adjoining area of the Atlantic Ocean (Figs. 2 and 3) averaged over the PBL height (taken to be 1.5 km) and over the cross section of the cell of $m \times n$ grid nodes with a horizontal step size of 250 km (Fig. 1). The calculation employed the data on annual emission of sulphurous gas as well as the climatic data on wind velocity and precipitation.

The calculated sulphurous gas concentration is shown in Figs. 2 (January) and 3 (July). Also shown are the fields of 850 hPa isobaric surface[1] that were used to calculate the PBL–average wind velocities at grid nodes along the coordinate axes.

As is seen from the figures, in both January and July, maximum level of pollution occurred in the PBL over the North–Eastern States of the U.S.A. in regions with developed industry, with the cell–average values of sulphurous gas concentration reaching 9 μg/m^3. Less polluted were the South–Eastern States, with concentration of about 3 μg/m^3. Over the Ocean, with an ecologically clean air, considerable concentration (up to 3–6 μg/m^3) was only found to occur in regions adjoining the North–Eastern States. In these regions, about 3000 km off–shore, pollutants were transported by strong (up to 12 m/s) westerlies. The sulphurous gas concentration did not exceed 1 μg/m^3 over the rest of the area of the Ocean.

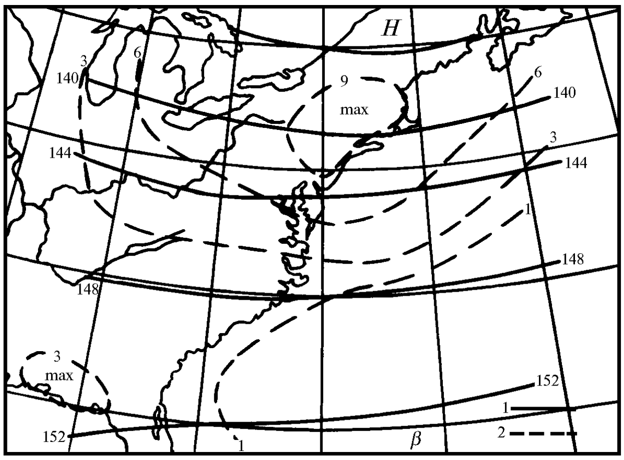

*FIG. 2. Reconstructed field of air pollution (*μg/m^3*) over Eastern States of the U.S.A. and adjoining area of the Atlantic Ocean: contours of* AT$_{850}$ (hPa) *(1) and sulphurous gas concentration (2) in January.*

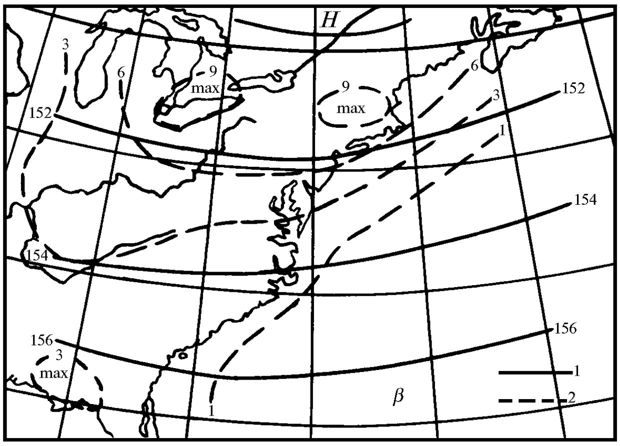

FIG. 3. Same as in Fig. 2, but for July.

Summarizing, with the method proposed above it is possible to estimate the level of pollution in any geographic region given the climatic data are available. The altitude– and area–average concentration so obtained characterizes some background level in the presence of sources of anthropogenic pollution in this region or nearby. More detailed patterns of pollution may be obtained with the use of local models or regional models with higher spatial resolution.

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