MATHEMATICAL SIMULATION IN ECOLOGY ON THE BASIS OF THE SIGN STREEM MODELS

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The mathematical model of the air transfer of the passive impurities is considered. As the apparatus of simulation we employed the language of the ideographical notios that admits the use of the automation system in designing models. We propose the criteria of dividing atmosphere into chambers and the algorithmical networks of the main units of the model of the ait transfer of impurities.

Air quality control is one of the most important aspects of the ecological situation monitoring. Air pollution takes place both from natural sources (volcanic emissions, forest fires, dust and sand, storms, dust inflows from space) and from the anthropogenic sources. Solution of the ecological problems needs for information about the air pollution coming from the anthropogenic sources first of all. They are the industial enterprises, energy installations (including nuclear ones), and transport. Therefore one of the modules of the ecology–economic models must be the module that describes the processes of the atmospheric pollution spread and transfer.

There is a lot of papers[1,3,4] concerning the problem of simulating the evolution of atmospheric pollutions from different sources and their precipitation onto the underlying surface. Since the atmospheric processes occur under combined influence of the natural and anthropogenic factors of different spatiotemporal scales, a rather complicated question arises on constructing mathematical models that take into account two contradicting circumstances simultaneously. On the one hand, a wide variety of the physical processes and perturbations of different kinds to be accounted for requires that the models developed should be physically complete and their discrete approximations must yield the required spatiotemporal resolutions. At the same time, such models must provide easy computer compatibility.

Experience of solving such problems shows that models based on systems of general (primitive) equations of the atmospheric hydrothermodynamics in nonadiabatic approximation with the account for moisture exchange processes and the processes of interaction between the atmosphere and thermally and orographically nonuniform underlying surface can be quite useful. Constructing such models is a very complicated problem even for professionals. Increasing the efficiency of the ecological researches and examinations of social development projects is very important today. Just for these reasons such ecological models must become a usual working instrument of corresponding specialists.

In this context we think that construction and performance of mathematical models should be based not on traditional mathematical descriptions of the processes under study and algorithmic languages of programming but on languages of knowledge representation oriented on an unskilled user. One of such languages, namely the language of algorithmic networks has been proposed in Ref. 2. It is an input language for the programming automation system SAPFIR. This language is oriented to describing ecological objects. In this case a mathematical model of a phenomenon under study is represented in the form of an oriented graph whose arcs correspond to the variables of an object simulated, and nodes correspond to the operators of the algorithmic networks language.

Here we propose a few–parametric model of the pollutions transfer by air (for a simplicity we consider only chemically passive impurities) in the form of algorithmic networks and intended for using as an individual unit in the contour of ecology–economic models.

It is known that the evolution of the aerosol formations in the atmosphere occurs due to advective transfer, large–scale (synoptical) vertical air motions, turbulent diffusion, convective air flows, the processes of washing out and sedimentation (i. e., by the processes of moist and dry sedimentation, respectively).

To mathematically describe the evolution processes of a chemically passive impurity with the mass concentration $S(x, y, z, t)$ we use the equation:

$$\frac{\partial s}{\partial t} + \mathbf{V} \operatorname{grad} s = \mu \, \Delta \, s + \frac{\partial}{\partial z} \nu \frac{\partial s}{\partial z} + f , \qquad (1)$$

where $\mathbf{V}$ is the vector of the motion velocity with the components u, v, and w; μ and ν are the coefficients of the turbulent exchange along the horizontal and the vertical directions; f is the function that describes the sources and sinks of a polluting substance.

The process of constructing a few–parametric model of the air transfer of impurities assumes that the problems to be solved are the following: determination of the structure of air volume division into uniform cells, choosing of the structure of a model for an individual cell, determination of the interactions between the cells, parametrization of the pollution sources, construction of the algorithmic networks, and assembling of the algorithmic model.

We will seek the solution of Eq. (1) in a limited spatial domain $G = \{0 \le x \le X,\ 0 \le y \le Y,\ 0 \le z \le Z\}$. The values X and Y are on the order of 10^2 km in the problems of local ecological monitoring. Since the aerosol of anthropogenic origin spreads within the planetary boundary layer of atmosphere, $Z \approx 1.5$ km. To derive unambignous solution of Eq. (1) we take into account the initial and boundary conditions.

The components of the motion velocity, the coefficients of the turbulent exchange, the sources and sinks of aerosol must be determined prior to calculations by Eq. (1). The models on the basis of solution of Eq. (1), must include a fairly great number of nodes (on

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the order of 10^4–10^5), otherwise the accuracy of calculations and agreement of our model with the physical pattern is poor. One can simplify the problem by introducing the cells (boxes) connected with each other. This enables one to simpler and more effectively take into account the main features of the horizontal transfer, the zones of condensation and precipitations, the thermal stability of atmosphere, and the relief peculiarities. In this case Eq. (1) is averaged over the volume of a cell.

Notice that it is too difficult to determine the objective criteria of the optimum, in a certain sense, division of the volume G under consideration into cells. Although it is clear that the structure of the spatial division of air volume under study, from the point of view of ecology, depends first of all on nonuniformity of the meteorological regime parameters along the horizontal and the vertical directions. It is apparent that the more nonuniform are the meteorological regime parameters, the greater is the number of cells required for the correct description of processes of the aerosol evolution in the atmosphere. In its turn, the nonuniformity of the meteorological parameters depends on the synoptical situation, the thermal and orographical nonuniformity of the region.

Generally the division into cells is performed on the basis of the objective analysis of the observational data of the wind velocity. Thus we can choose the cells where the speed and direction of the wind are uniform.

In dividing the atmospheric volume under study into cells it is advisable to use the two–dimensional, x, y, approximation that enables us to average Eq. (1) over a vertical path in a special way. It is conditioned by the fact that the variability of the meteorological parameters along a vertical path exceeds by three to four orders of magnitude the variability along a horizontal path. Inside the boundary layer we can choose the surface sublayer (the layer of constant turbulent fluxes of heat, moisture, and momentum). Therefore the upper and lower boundaries of the atmospheric surface layer may be the boundaries of the cells.

Above the surface layer the inverse distribution of temperature very often takes place. Inversion, as known, prevents penetration of impurities into the above layers. Therefore it is reasonable to take the levels corresponding to the lower and upper boundaries of the inversion layer as the cells boundaries.

Above the layer or in case of its absence above the surface layer the division into cells needs to be done in accordance with the following circumstances.

1) there takes place a smooth turn of the wind direction at an angle of 30–35° within the boundary layer of the atmosphere;

2) the lapse rate of the wind velocity modulus along a vertical path has the order of 10^{-2};

3) the accuracy of measurements of the wind characteristics amounts to nearly 20–25%;

4) the influence of the underlying surface and the variability of meteorological parameters is most essential in the lower half of the atmospheric boundary layer.

Thus the cells sizes along the vertical path must be different: the vertical dimensions of the cells for the lower half of the boundary layer (up to the level of 500 m) must be within 50–150 m and 300 m and more for the upper half. Since the accuracy of the measurement of wind characteristics is poor, it is hardly reasonable to take more than 10 cells along a vertical path.

Dividing into cells along a horizontal direction must be done taking into account the rate of advective transfer (the higher is the rate, the greater horizontal dimensions of the cells are required) and the rate of sedimentation.

The dimensions of the cells along a horizontal direction may be different. In immediate vicinity of a source of pollution the cells dimensions can be essentially smaller than far from it. Since we consider the task of propagation of impurities on a scale of $10^2 \times 10^2$ km^2 and taking into account the characteristic rate of advection, 10 m/s, the cells dimensions along the horizontal direction must be ≈10×10 km^2 for the light impurities and 1×1 km^2 for heavy ones.

So at first sight the total number of cells should be on the order of 10^3. However in reality, when constructing the model of transfer, the number of cells is decreased by an order at least. This is because the advective transfer dominates over the turbulent diffusion and so there is no sense to introduce cells in the direction perpendicular to the direction of the advective transfer. Because of large size of cells it is necessary to provide the possibility of describing the distribution of the impurity concentration inside each cell in more detail.

Averaging Eq. (1) over a cell volume V

$$\tilde{s} = \frac{1}{V} \int \int_{V} \int s \, \mathrm{d}x \, \mathrm{d}y \, \mathrm{d}z \, , \tag{2}$$

we can obtain a system of differential equations that describes the evolution of the field of impurities.

Rewrite Eq. (1) in the divergence form taking into account sedimentation and the washing out:

$$\frac{\partial s}{\partial t} + \mathrm{div}\, \mathbf{V}\, s = \frac{\partial}{\partial z} \nu \frac{\partial s}{\partial z} + \mu \, \Delta \, s + Q + f \, , \tag{3}$$

where Q is the summand that describes the moist and dry sedimentation.

Integrating Eq. (3) over the height from the lower level z_{low} to the upper level z_{up} we have

$$\frac{\partial}{\partial t} \int_{z_{\mathrm{low}}}^{z_{\mathrm{up}}} s \, \mathrm{d}z + \int_{z_{\mathrm{low}}}^{z_{\mathrm{up}}} \mathrm{div}\, \mathbf{V}\, s \, \mathrm{d}z =$$

$$= \int_{z_{\mathrm{low}}}^{z_{\mathrm{up}}} Q \, \mathrm{d}z + \int_{z_{\mathrm{low}}}^{z_{\mathrm{up}}} \frac{\partial}{\partial z} \nu \frac{\partial s}{\partial z} \, \mathrm{d}z + \mu \, \Delta \int_{z_{\mathrm{low}}}^{z_{\mathrm{up}}} s \, \mathrm{d}z + \int_{z_{\mathrm{low}}}^{z_{\mathrm{up}}} f \, \mathrm{d}z \, . \tag{4}$$

Let us consider that the components of the velocity of horizontal transfer inside the cell along the height are constant. Introducing the integral intensity of aerosol, source, and sinks

$$\overline{s} = \int_{z_{\mathrm{low}}}^{z_{\mathrm{up}}} s \, \mathrm{d}z \, , \; \overline{f} = \int_{z_{\mathrm{low}}}^{z_{\mathrm{up}}} f \, \mathrm{d}z \, , \; \overline{Q} = \int_{z_{\mathrm{low}}}^{z_{\mathrm{up}}} Q \, \mathrm{d}z \, , \tag{5}$$

we obtain

$$\frac{\partial \overline{s}}{\partial t} + \frac{\partial}{\partial x} (u \, \overline{s}) + \frac{\partial}{\partial y} (v \, \overline{s}) + w \, s \Bigg|_{z=z_{\mathrm{low}}}^{z=z_{\mathrm{up}}} =$$

$$= \overline{Q} + \nu \frac{\partial s}{\partial z} \Bigg|_{z=z_{\mathrm{low}}}^{z=z_{\mathrm{up}}} + \overline{f} + \mu \, \Delta \, \overline{s} \, , \tag{6}$$

We also assume that the horizontal speed inside the cells is constant. Then

$$\frac{\partial \bar{s}}{\partial t} + u\frac{\partial \bar{s}}{\partial x} + v\frac{\partial \bar{s}}{\partial y} + w\,\bar{s}\,\Bigg|_{z=z_{\rm low}}^{z=z_{\rm up}} =$$

$$= \bar{Q} + \nu\frac{\partial \bar{s}}{\partial z}\,\Bigg|_{z=z_{\rm low}}^{z=z_{\rm up}} + \mu\,\Delta\,\bar{s} + \bar{f}\ . \qquad (7)$$

Equation (7) is the main prognostic equation that describes the evolution of the impurity field. To solve it we have know the following information:

a) the information about the pollution sources (localization, intensity);

b) the calculated values of the coefficients of vertical and horizontal turbulent exchange;

c) the values of the components of the velocity vector;

d) the numerical value of the summand that describes the moist and dry sedimentation;

e) the initial field of the impurity concentration and the aerosol microphysical characteristics.

We solved Eq. (7) by the method of splitting over the physical processes, i.e., at each step in time one solves the following three problems:

1) the problem of the advective transfer

$$\frac{\partial \bar{s}}{\partial t} + u\frac{\partial \bar{s}}{\partial x} + v\frac{\partial \bar{s}}{\partial y} = 0\ ; \qquad (8)$$

2) the problem of the turbulent exchange

$$\frac{\partial \bar{s}}{\partial t} = \mu\,\Delta\,\bar{s} + \frac{\partial}{\partial z}\,\nu\,\frac{\partial s}{\partial z}\ ; \qquad (9)$$

3) the problem that describes the sources and sinks of aerosol

$$\frac{\partial \bar{s}}{\partial t} + w\,\bar{s}\,\Bigg|_{z=z_{\rm low}}^{z=z_{\rm up}} = \bar{Q} + \bar{f}\ . \qquad (10)$$

In the model of air transfer of impurities the atmosphere can be represented in the form of a parallelepiped divided into cells. Those cells whose faces are unfair with the limits of the calculation domain we call the unified ones.

Among the variables that are necessary for the impurity concentration in the unified chamber to be calculated are: the values of the impurity concentration in the six adjacent cells, the values of the velocity components of motion averaged over the volume of a cell, the coefficient of washing out, the coefficients of turbulence, and the rate of gravitational sedimentation. For the nonunified cells this list will be changed with regard to the boundary conditions.

Before we form the algorithmic network of model the equations (8)–(10) need to be reduced to the finite–differential form. Figures 1–4 show the algorithmic networks of the main units of the model of air transfer (i, j, and l are the cells indices with respect to x, y, and z axes).

The results of the test numerical experiments showed high efficiency of this mathematical apparatus of describing and forecasting air pollutions.

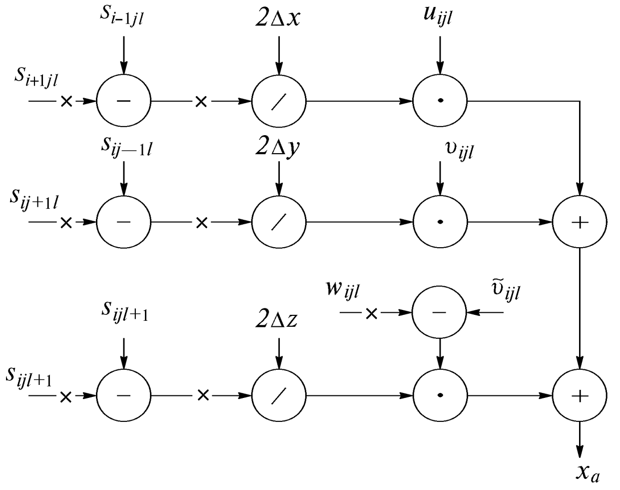

FIG. 1. The algorithmic network of the advective–convective block.

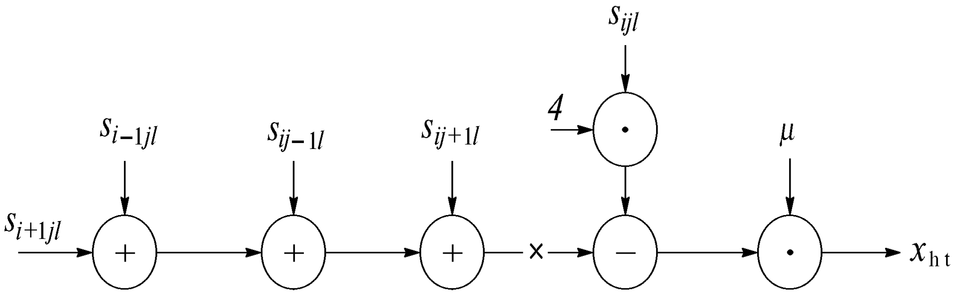

FIG. 2. The algorithmic network of the block of the horizontal turbulent diffusion.

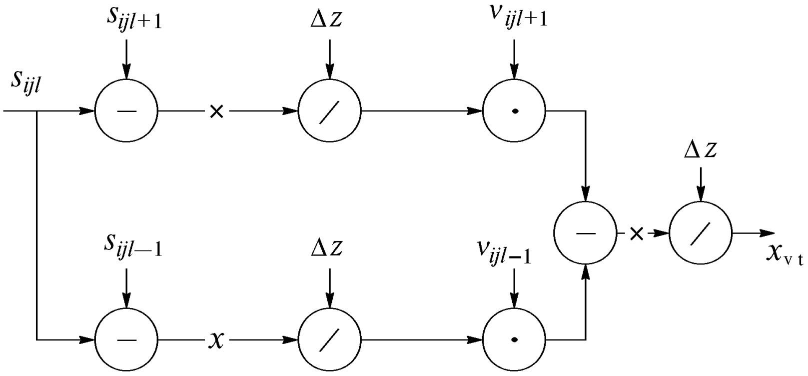

FIG. 3. The algorithmic network of the block of the vertical turbulent diffusion.

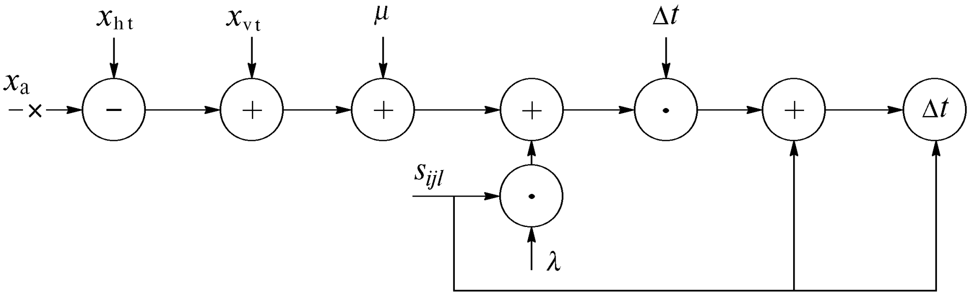

FIG. 4. The algorithmic network of the calculational block of the concentration of impurity by the time t + Δt.

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