VARIATIONAL ALGORITHMS FOR SIMULATING THE AEROSOL AND HYDRODYNAMIC FIELDS IN THE ATMOSPHERE

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We propose, when tackling the problem of aerosol transfer, within an arbitrary time interval, to replace it by a problem of optimal control. The cost functional is chosen, for that case as deviation of the initial solution from the solution of a problem with known diffusion. In so doing, we consider a meteorological model that is based on the concept of artificial compressibility. The results obtained from experiments qualitatively well agree with the theory and data of observations available.

1. INTRODUCTION

Aerosol transfer in the atmosphere is traditionally described by a convection-diffusion equation. Simulating aerosol transfer under conditions of dominating convection requires for use of numerical procedures that provide for suppressing the oscillations that may appear in calculations of the aerosol wave near its front.

Here we consider the approach that enables one, within the same frameworks, to suppress the non-monotonic features and assimilate an additional information (if any) about a solution to the transfer equations. At the same time, we consider in this paper only the variational aspect of the problem on making the solution monotonic.

The idea of applying the apparatus of adjoint equations to meteorological problems has first been proposed by Marchuk.[1] In the context of variation assimilation of the data, the adjoint equations can be used to calculate gradient of the cost functional with respect to the initial data of the model. This gradient is then used to make the "descent steps," in the space of the initial data, and the iteration process is repeated until the initial data are approximated quite satisfactorily to minimize the cost functional. The use of the adjoint equations in such an approach has been proposed by Penenko.[2] Since then many authors have been using this approach in the context of data assimilation (see, for instance, Ref. 3).

Knowledge of the spatial and time behaviors of the meteorological quantities is very important when solving problems of the aerosol transfer and transformations in the atmosphere. Large variations of these fields are difficult to be determined only from measurements, in the zones of complicated processes. Meteorological models have become an important tool for extracting that type of hard-to-obtain information.[4]

Most of the modern non-hydrostatic models use the so-called "inflexible" approximation in which sound waves are filtered using a modified equation of discontinuity. As a result, the pressure can not already be determined explicitly, while being obtained using a complicated differential equation. As a consequence, one must solve this equation at every time step to modify the pressure field. So, it is much more difficult to numerically treat an inflexible system as compared with the treatment of a system of equations that is obtained for the hydrostatic case.[9] In recent years, the development of numerical methods has made it possible to create non-hydrostatic models[10–12] that do not filter sound waves.

It is evident that a numerical model that could provide for a detailed description of atmospheric processes must not only provide for obtaining exact solutions of the relevant mathematical equations. It also must involve a realistic representation of the Earth's surface. In this connection, coordinate systems that trace the surface are most widely spread in use. After making relevant substitution of variables, the domain where the calculations are to be done becomes simple and can easily be discretized. However, thus transformed equations are more complicated. Generally speaking, the transforming functions must be sufficiently smooth, that means that one have restrict oneself to only a smooth idealization of a real surface.[9]

To obtain hydrostatic fields that make up the backbasic for aerosol spread, we consider in this paper a three-dimensional meteorological model that is based on the method of artificial compressibility (earlier versions are presented in Refs. 6 and 7). The method of artificial compressibility has been proposed by Yanenko[13] and Chorin[14] and then successfully applied to solving different problems in fluid dynamics. Using this method one can considerably simplify in a non-hydrostatic model the process of solving the equation for pressure in the regions of complicated scenarios. The finite-difference and finite-element variants of the model are used for a surface with small and large spatial gradients, respectively.

2. AEROSOL TRANSFER AND DIFFUSION

The convection-diffusion equation for the transfer of a substance in the atmosphere has the following form[4]:

$$\frac{\partial c}{\partial t} = \nabla\,(\mathbf{D}\,\nabla c - \mathbf{v}c) - \lambda c + q. \tag{1}$$

Here $c(\mathbf{x}, t)$ is the concentration of the substance; $\mathbf{D}(\mathbf{x}, t)$ is the variance tensor; $\mathbf{v}(\mathbf{x}, t)$ is the wind velocity; $\lambda(\mathbf{x}, t)$ describes chemical reactions; $q(\mathbf{x}, t)$ is the term of a source or a sink, $\mathbf{x} \in R^d$, $d = 1, 2, 3$.

Suppose that the problem (1) has the following spatial form:

$$\frac{\mathrm{d}\varphi}{\mathrm{d}t} = H(\varphi), \tag{2}$$

where H is some regular operator in the space. For instance, one can use central differences to obtain high spatial approximation. If the convection dominates over the diffusion, use of central differences lead to appearance of strong oscillations in the calculated numerical solution.

Let there be some supplementary information on the behavior of the physical solution in the form of "observations" $\hat\varphi(t_i)$, and $\hat\varphi(t_1),\ldots,\hat\varphi(t_n)$ let also be found at times $t_1 <\ldots< t_n$. We seek a solution $\varphi(t)$ that minimizes the functional

$$J[\varphi(t)] = \sum_{i=1}^{n} [\varphi(t_i) - \hat\varphi(t_i),\, \varphi(t_i) - \hat\varphi(t_i)] +$$
$$+ \sum_{i=1}^{n} [\nabla(\varphi(t_i) - \hat\varphi(t_i)),\, \nabla(\varphi(t_i) - \hat\varphi(t_i))],$$

where [,] is the scalar product.

Let us consider then the linearized equation for perturbations

$$\frac{\mathrm{d}}{\mathrm{d}t}\,\delta\varphi = A(t)\,\delta\varphi \tag{3}$$

with the initial condition $\delta\varphi(t_1)$ and the adjoint differential equation

$$\frac{\mathrm{d}}{\mathrm{d}t}\,\delta^*\varphi = A^*(t)\,\delta^*\varphi. \tag{4}$$

Here the operator $A^*(t)$ is the complex conjugate to A.

One cycle of calculations of the functional gradient with respect to the initial field contains: (1) one calculation of the direct model; (2) one calculation of the adjoint model in the direction opposite to that for determining the gradient.

Having obtained the gradient, one can use a descent algorithm to obtain a correction to the initial conditions. The approximations obtained from the following series

$$c = C_0 + \sum_{k=1}^{\infty} C_k/(\mathrm{Re})^k, \tag{5}$$

where Re is Reynolds number in our problem, are used as the "observations". This series leads to a sequence of hyperbolic equations that can be solved, for instance, by the method of characteristic curves.

The idea of using this series in a problem of optimal control was proposed in Ref. 5, though in actual calculations a certain variant of the front fitting was used as a sort of restriction. In this paper we generalize this method to develop a unified approach that could be applicable to finite-difference, finite-element, or spectral approximations.

Let us consider the results calculated for the case of a passive admixture transfer over a mountain ridge, as an example. The shape and dimensions of the ridge, as well as the triangulation of the calculation domain is shown in Fig. 1.

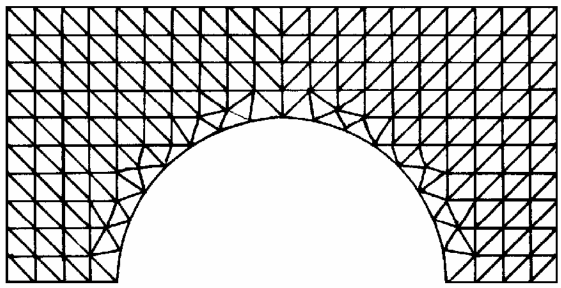

FIG. 1. Triangulation of the domain.

The domain has total height of 500 m, horizontal extension of 10 km, and the height of the hill of 300 m. The calculation grid consists of 296 triangular elements; horizontal and vertical dimensions of the grid cell are 500 and 50 m, respectively.

Figure 2 presents the field of the admixture concentration at a horizontal wind speed of 10 m/s and the vertical one of 3 m/s. The horizontal and vertical coefficients of diffusion are 100 and 10 m/s, respectively. The source of the emission with the normalized intensity of 1 is situated at the left boundary at a height of 100 m.

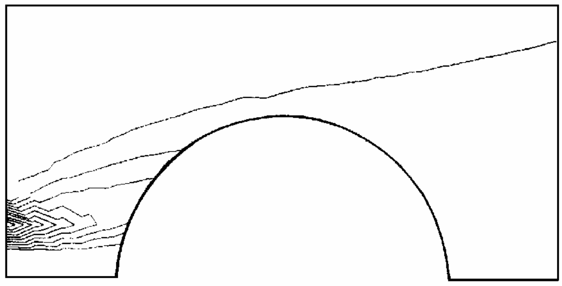

FIG. 2. The field of the admixture concentration.

3. THE METEOROLOGICAL MODEL

The basic equations of motion, heat, humidity, and discontinuity, which are presented here in a three-dimensional form are as follows:

$$\frac{\mathrm{d}U}{\mathrm{d}t} + \frac{\partial P}{\partial x} + \frac{\partial P}{\partial z} = f_1\,(V - V_{\mathrm{g}}) - f_2\,W + R_u,$$

$$\frac{\mathrm{d}V}{\mathrm{d}t} + \frac{\partial P}{\partial y} + \frac{\partial P}{\partial z} = -\,f_1\,(U - U_{\mathrm{g}}) + R_v,$$

$$\frac{\mathrm{d}W}{\mathrm{d}t} + \frac{\partial P}{\partial z} + \frac{gP}{C_{\mathrm{s}}^2} = f_2\,U + g\,\frac{\bar{\rho}\,\theta'}{\bar{\theta}} + R_w,$$

$$\frac{\mathrm{d}\theta}{\mathrm{d}t} = R_\theta,\ \frac{\mathrm{d}s}{\mathrm{d}t} = R_{\mathrm{s}},$$

$$\frac{1}{C_{\mathrm{s}}^2}\frac{\partial P}{\partial t} + \frac{\partial U}{\partial x} + \frac{\partial V}{\partial y} + \frac{\partial W}{\partial z} = \frac{\partial}{\partial t}\left(\frac{\bar{\rho}\,\theta'}{\bar{\theta}}\right).$$

Here $U = \bar{\rho}u$, $V = \bar{\rho}v$, $W = \bar{\rho}w$, $P = p'$, where p', θ' are the deviations of pressure $\bar{p}$ and potential temperature $\bar{\theta}$ from the basic state; s is the specific humidity; C_{s} is the speed of sound; u_{g}, v_{g} are geostrophic wind components representing the synoptic part of the pressure; f_1, f_2 are Coriolis parameters; g is the acceleration of gravity.

For an arbitrary function φ

$$\frac{\mathrm{d}\varphi}{\mathrm{d}t} = \frac{\partial\varphi}{\partial t} + \frac{\partial u\varphi}{\partial x} + \frac{\partial v\varphi}{\partial y} + \frac{\partial w\varphi}{\partial z}.$$

The terms R_u, R_v, R_w, R_θ, R_s describe the processes on a sub-grid scale. To parameterize the turbulence, we use a simple scheme based on calculations of the Blacadar mixing path.[8] Usual logarithmic profiles of wind between the surface and first layer of the atmosphere are being estimated. We take 0.1 m for the roughness length.

For the upper boundary, we take the condition

$$w = 0,\ u = u_g,\ \ v = v_g,\ \ \theta = \theta_t,$$

where θ_t is the constant value that is set by the basic state.

For the lower boundary, we take that

$$w = 0,\ \theta = \theta_s(x,\ y)$$

that means that the same value as of the basic state at the same level. Turbulent fluxes through the surface layer are determined using Monin-Obukhov similarity theory.[8]

In this paper, side boundaries are defined from the condition that normal derivatives equal zero for all the calculated fields.

Both the finite-difference and finite-element variants of the model essentially use the method of artificial compressibility for equations of the Navier-Stokes type.[13–14] The finite difference variant of calculations is described in Ref. 6. As to the finite-element case, the spatial discretizing of the initial equations is based on the method of weighed residuals. The dependent variables are represented in the form

$$P = \sum_{i=1}^{m} \beta_i(\bar{\mathbf{x}})\ P_i(t),$$

$$\varphi = \sum_{i=1}^{n} \alpha_i(\bar{\mathbf{x}})\ \varphi_i(t),$$

where φ can be U, V, W, θ, or s. Here m points in a discrete domain are for P and n points for other variables. The approximating functions $\alpha_i(\bar{\mathbf{x}})$ are piece-wise continuous bilinear polynomials (for the 2D variant of the model considered here), the functions $\beta_i(\bar{\mathbf{x}})$ for P are piece-wise constant.

We consider here the Arakawa grid, in which P is determined at the center of each element. After substitution into the initial equations, multiplying each equation by the corresponding weighting function (β_i for the equation of discontinuity and α_i for other equations), and integrating by parts, we obtain a non-linear system of ordinary differential equations of the first order. The diffusion terms are realized by 2×2 Gaussian quadrature formulas, all the other integrals are represented by single-point formulas.

Discretizing in time is performed in a standard way into the transfer and adaptation stages.[6] At the first stage, the schemes of Krank-Nicholson type are being applied. At the adaptation stage, the equation for pressure is realized by the direct method combined with the time iterations.[6]

Let us present the results of the finite-difference experiment for a meteorological flow over an isolated hill. The hill of a 500 m height is situated at the center of a 10×10 km area. The top of the area is at 5 km. The geostrophic flow is spread from west to east at a speed of 5 m/s. The standard atmospheric stratification with the gradient of 3.5 K/km is taken as the basic state. The absorbing layer is situated above 1500 m. The calculation grid consists of 31×31×16 points with the horizontal size of 333 m and variable vertical size.

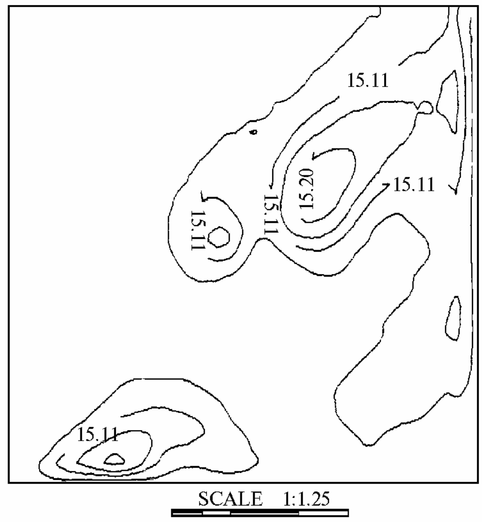

FIG. 3. Potential temperature at the level of 20 m.

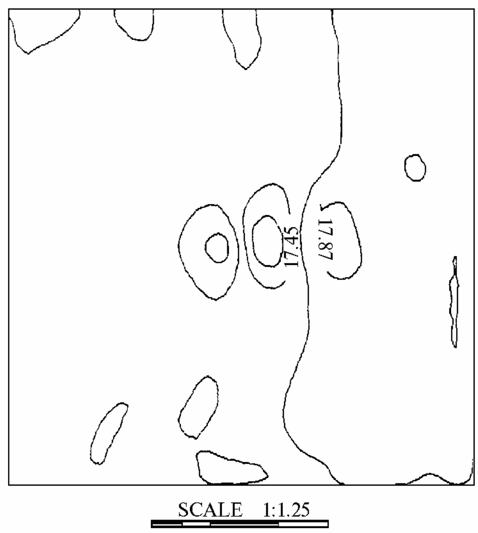

FIG. 4. Potential temperature at the level of 400 m.

Figures 3 and 4 demonstrate horizontal sections of the potential temperature at the levels of 20 and 400 m respectively. The flow tends to turn left at low levels. At the same time, the flow is almost symmetric at the upper levels. The results of these model experiments qualitatively agree with the theory[15] and data of observations available.

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