Transport of aerosols over complex terrain on small scales: semi-Lagrange and random walk methods

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Received November 9, 2000

A mesoscale meteorological model is used for mathematical simulation of aerosol spreading under conditions of a complex terrain. Aerosols are transported against the background of meteorological fields calculated by this model. Two approaches are discussed: the semi-Lagrange method for calculation of aerosol advection and the simple model of random walk of particles. An example of calculation of aerosol transport over a steep hill is presented. In this example, the temperature field is calculated by the first method, and the aerosol transport is calculated by the second method. The obtained pattern of aerosol sedimentation agrees qualitatively with the existing theory.

Introduction

There exist a great number of practical and theoretical problems dealing with transport of atmospheric aerosols over a region having a complex irregular structure. The pollutant spreading under urban conditions, simulation of microclimate, and others are among such problems. The existing observational network is usually sparse, and obtained data are not always representative for a region with a complex structure.

In this connection, mathematical models of atmospheric processes are necessary tools for obtaining missing information.[1] Meteorological fields obtained using these models serve a background for calculation of advection and diffusion of aerosol particles.

Unlike many usual methods for calculating the spatial and temporal distributions of meteorological elements, here we discuss two methods dealing with the behavior of individual aerosol particles. One of the existing approaches to calculation of large-scale advection is the so-called semi-Lagrange method.[2,3] This method minimizes computational errors, and in this sense it has an advantage over the traditional Euler approach. Section 1 presents a version of this method for the case of interpolation schemes of the high order of approximation. Then this method is used for calculation of the temperature field in the mathematical model of atmospheric dynamics described briefly in Section 3.

Another popular method of calculating particle motion is the random walk method or method of Lagrange diffusion.[4] Models of random walk of particles are free of the problems of computational errors and algorithm stability and have some technical advantages. In Section 2 we describe schematically a simple model of Lagrange diffusion. This model is used in Section 4 for simulating the passive aerosol spread over a steep hill. The equations of the model for meteorological background are given in Section 3.

1. Semi-Lagrange advection of aerosol

The considered method for calculating advection at aerosol transport consists of two stages.

1. Determination of aerosol particle exit points, i.e., the points from which the information on aerosol distribution is delivered to the next time step;

2. Interpolation of the values of f from the closest nodes of the spatial grid to the particle exit points:

$$x_D = x - \int v \mathrm{d}t; \quad f(x,\ t + \Delta t) = f(x_D,\ t),$$

where Δt is a time step; x_D is an exit point. The order of interpolation determines the accuracy of the method. In this paper we use the third order scheme by the reasons that will be discussed below. This scheme is constructed in the following way. The arbitrary function f at a node of the difference grid is expanded into a series accurate to the terms of the fourth order. Free coefficients of this expansion are determined through the values of the function at the closest grid nodes. Let us denote $\lambda = (x_D - x_i)/\Delta x$. Here Δx is a spatial step. Having solved the obtained system of linear equations, we derive

$$f(t + \Delta t) = f_i\,(1 - \lambda/2 - \lambda^2 + \lambda^3/2) +$$
$$+ f_{i+1}(\lambda + \lambda^2/2 - \lambda^3/2) + f_{i+2}\,(-\lambda/6 + \lambda^3/6) +$$
$$+ f_{i-1}\,(-\lambda/3 + \lambda^2/2 - \lambda^3/6).$$

Experiments with the schemes of different orders allow the following conclusions:

1. Schemes of the first order have high numerical diffusion.

2. Schemes of the second order are nonmonotone and have small-scale wavy structure.

3. In the third order schemes under consideration, both these types of errors are suppressed to high degree.

0235-6880/00/12 1048-03 $02.00

4. The schemes of higher orders lead to insignificant gain in the quality of solution with significant increase of computational expenses.

2. Model of random walk

The simple model of Lagrange diffusion[4] was chosen for calculation of aerosol transport and diffusion. This model is attractive due to its mathematical simplicity and flexibility.

At the time $t + \Delta t$ individual aerosol particles have the coordinates:

$$x_i\,(t + \Delta t) = x_i(t) + U_i(t)\,\Delta t, \quad i = 1,\ 2,$$

$$x_3\,(t + \Delta t) = x_3(t) + (U_3(t) - V_{\rm sed})\,\Delta t,$$

where x_i is the coordinate of the ith particle; U_i is the full speed of the particle; $V_{\rm sed}$ is the sedimentation rate.

The speed U_i can be divided into the mean speed u_i, which follows from calculation by the meteorological model (see the next section), and the turbulent component u_i'. This component is calculated as follows:

$$u_i'(t + \Delta t) = R_{{\rm L}_i}(\Delta t)\,u_i'(t) + (1 - R_{{\rm L}_i}(\Delta t)^2)^{1/2}\,\sigma_{u_i}\,\Psi;$$

$$R_{{\rm L}_i}(\Delta t) = \exp\,(-\,\Delta t/T_{{\rm L}_i}).$$

Here Ψ is a random-number generator for the Gaussian distribution; $T_{\rm L}$ and $R_{\rm L}$ are Lagrange time scales and autocorrelations;

$$\sigma_u = (2m_1\,E)^{1/2},\ \sigma_v = (2m_2\,E)^{1/2},\ \sigma_w = (2m_3\,E)^{1/2}.$$

For three types of stratification:

$$\frac{\partial\theta}{\partial z} \le -\,0.5\ K/100\ {\rm m},\ \left|\frac{\partial\theta}{\partial z}\right| < 0.5\ K/100\ {\rm m},$$

$$\frac{\partial\theta}{\partial z} \ge 0.5\ K/100\ {\rm m},$$

we use the following sets of coefficients:

$$m_1 = 0.4,\ 0.54,\ 0.54;\ m_2 = 0.30,\ 0.30,\ 0.37;$$

$$m_3 = 0.30,\ 0.16,\ 0.09;$$

$$T_{{\rm L}_i} = K/\sigma_{u_i}^2.$$

Unlike Ref. 4, we have not a specialized equation for calculation of the kinetic energy of turbulence. Therefore, we find it from the equation

$$K = l\,\sqrt{cE}\ ,$$

where c is an empiric constant, $c = 0.2$ (Ref. 4).

The diffusion coefficient K is calculated using the model of atmospheric thermodynamics.

3. Model of atmospheric background

To calculate meteorological fields, we use the following equations of atmospheric dynamics:

$$\frac{{\rm d}U}{{\rm d}t} + \frac{\partial P}{\partial x} + \frac{\partial(G^{13}\,P)}{\partial\eta} = f_1\,(V - V_{\rm g}) - f_2\,W + R_u,$$

$$\frac{{\rm d}V}{{\rm d}t} + \frac{\partial P}{\partial y} + \frac{\partial(G^{23}\,P)}{\partial\eta} = -\,f_1\,(U - U_{\rm g}) + R_v,$$

$$\frac{{\rm d}W}{{\rm d}t} + \frac{1}{G^{1/2}}\frac{\partial P}{\partial\eta} + \frac{gP}{C_{\rm s}^2} = f_2 U + g\,\frac{G^{1/2}\,\bar\rho\,\theta'}{\theta} + R_w;$$

$$\frac{\partial\theta}{\partial t} = R_\theta;\ \ \frac{{\rm d}s}{{\rm d}t} = R_s;$$

$$\frac{1}{C_{\rm s}^2}\frac{\partial P}{\partial t} + \frac{\partial V}{\partial y} + \frac{\partial}{\partial\eta}\left(G^{13}\,U + G^{33}\,V + \frac{1}{G^{1/2}}\,W\right) = \frac{\partial}{\partial t}\left(\frac{G^{1/2}\,\bar\rho\,\theta'}{\theta}\right);$$

$$U = \bar\rho\,G^{1/2}\,u;\ \ V = \bar\rho\,G^{1/2}\,v;\ \ P = \bar\rho\,G^{1/2}\,p',$$

where p' and θ' are deviations of the pressure $\bar p$ and the potential temperature $\bar\theta$ from the ground state; s is specific humidity; $C_{\rm s}$ is the speed of the sonic wave; $u_{\rm g}$ and $v_{\rm g}$ are the geostrophic wind components representing the synoptic part of the pressure; f_1 and f_2 are Coriolis parameters; g is a gravitational constant; G are Christoffel symbols.

For the arbitrary function φ

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

The terms R_u, R_v, R_w, R_θ, and R_s describe the processes of the subgrid scale in terms of the K-theory. The turbulent exchange coefficients are calculated as:

$$K_m = \begin{cases} l^2\,[(\mathbf{D}^2)\,(1 - {\rm Ri})/2]^{1/2} & \text{at Ri} < 1,\\ 0 & \text{at Ri} \ge 1.\end{cases}$$

Here $\mathbf{D} = \nabla\mathbf{u} + \mathbf{u}\nabla$.

The mixing way l at every grid point is taken as the shortest distance to obstacles in all directions. The local Richardson number Ri is used in the form

$${\rm Ri} = \frac{g}{\theta}\,\frac{\partial\theta/\partial\eta}{\mathbf{D}^2/2}\ .$$

A more detailed description of this model can be found, for example, in Refs. 5 and 6.

4. Aerosol spreading over a hill

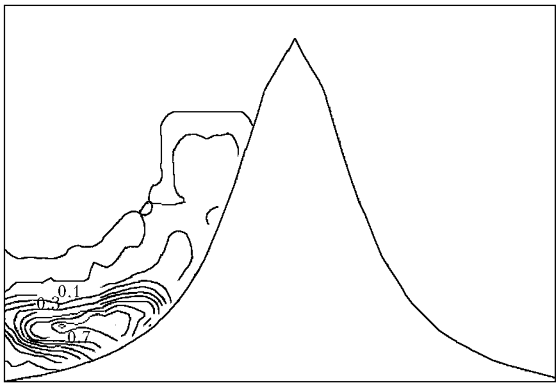
In this section, we present the results on aerosol transport over a steep hill. In this case, the semi-Lagrange method is used for calculating the temperature field in the model of atmospheric dynamics from Section 3. The aerosol transport is simulated by the random walk method.

A hill 500 m high is situated at the center of a region 10 × 10 km. The region height is 5 km. The geostrophic flow comes from the west, $u_{\rm g} = 5$ m/s, $v_{\rm g} = 0$.

The standard atmospheric stratification 3.5 K/km is taken as the ground state.

The absorbing layer is situated at the altitude of 1500 m. The computational grid consists of 31 × 31 × 16 points. The horizontal step of the grid is $\Delta x = \Delta y = 333$ m; the vertical step increases with height. The height of the hill increases gradually from zero for the first 15 min. The aerosol source of 5000 particles is to the east of the hill; the particle sedimentation rate is taken equal to 2 cm/s.

Figures 1 and 2 illustrate the aerosol motion over the hill. The east-to-west vertical sections of the hill are shown there.



Scale 1:1.188

Fig. 1.

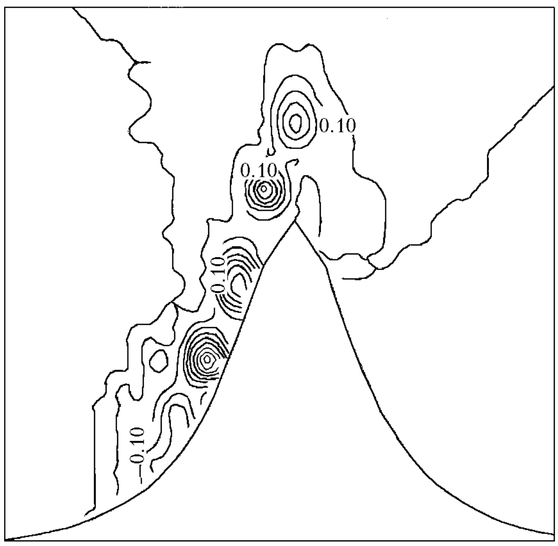


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Fig. 2.

Figure 3 shows the aerosol concentration on the surface within 20 min of physical time (top view). The aerosol flow is markedly shifted in the northeastern direction, in spite of the fact that the initial parameters of the problem are symmetric about the east-to-west direction. Such a pattern of spreading is in agreement with the existing theoretical concepts, because the meteorological fields in this situation are shifted due to the Coriolis force.[7]

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Fig. 3.

The results of these and similar test calculations allow the conclusion that the semi-Lagrange method in combination with the method of Lagrange diffusion can be used for numerical simulation of aerosol spreading over a region with complex terrain.

Acknowledgments

The author is thankful to M. Pynzar, who took part in programming and computing by the model of Lagrange diffusion.

This work was reported at VI Workgroup on Siberian Aerosols in Tomsk in November 1999.

This work was partially supported by the Russian Foundation for Basic Research (Grants No. 98–05–65318 and No. 99–07–90422) and the Integration Grant SB RAS–2000 No. 64.

References

1. V.V. Penenko and A.E. Aloyan, *Models and Method for Problems of Environmental Protection* (Nauka, Novosibirsk, 1985), 256 pp.
2. T. Ritchie, Mon. Wea. Rev. **115**, 135–146 (1987).
3. V.N. Krupchatnikov and A.A. Fomenko, "*ECSib semi-Lagrange semi-implicit scheme*," Preprint No. 1105, Institute of Computational Mathematics and Mathematical Geophysics, Novosibirsk (1997), 21 pp.
4. G. Gross, H. Vogel, and F. Wippermann, Atmos. Environ. **21**, 483–490 (1987).
5. M.S. Yudin, Bull. Nov. Comp. Center. Num. Model Atmosph. **2**, 101–107 (1995).
6. M.S. Yudin and K. Vilderotter, Atmos. Oceanic Opt. **11**, No. 10, 973–976 (1998).
7. E.E. Gossard and U.H. Hook, *Waves in the Atmosphere* [Russian translation] (Mir, Moscow, 1978), 532 pp.