Study of mesoscale transport of impurities based on models of Euler and Lagrange types

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We present a complex of models of mesoscale transport of impurities including the deterministic model in terms of Euler formulation and the deterministic-stochastic model formulated in the frameworks of Lagrange approach. Some results of comparative experiments on modeling the impurity transport within the regions having complicated geometry are presented in the paper.

Introduction

Investigations into the development of mathematical models and techniques for describing the transport, diffusion, and turbulent exchange of impurities in gaseous and aerosol states have been actively carried out since the beginning of XX century. By now, considerable experience has been accumulated in using deterministic and stochastic models for diagnostics and forecast of air quality changes due to natural and anthropogenic effects. Quite wide reviews of principal approaches to the solution of this class of problems are given in Refs. 1–3 and publications cited therein. These approaches can be conventionally categorized in accordance with the models used: 1) models of Euler type, where equations of advection–diffusion type are integrated over spatiotemporal grids of a preset structure and 2) models of Lagrange type, where advection and diffusion submotions of impurity particles are calculated in different ways on some gridless structures, evolutionary changeable in space and time depending on the behavior of the carrier medium.

Note, that these approaches are not alternative. They differ in system organization of algorithms and, actually, complement each other. Each of them has its own advantages and disadvantages and fields of application. Therefore, hybrid systems are of interest, which combine the most important advantages of both approaches. A system of such a type is being developed at the Institute of Computational Mathematics and Mathematical Geophysics SB RAS. It is based on variational principles with the use of direct and conjugate problem and methods of the sensitivity theory for deterministic and deterministic-stochastic models of transport and transformation of impurities.[4–6] This work presents one of its modifications for the solution of 4D mesoscale impurity transport problems in the forward modeling mode. Its key elements are deterministic model in terms of Euler and deterministic-stochastic model of Lagrange type. To calculate parameters of hydrodynamic background of the atmosphere as a carrier medium a non-hydrostatic mesoscale model of atmospheric dynamics is used in the regions of a complex terrain.[7,8]

The analysis of validity and comparison of two models were based on the solution of the problem of passive impurity emission.

1. Problem statement

Thus, in this paper we consider a model of a passive impurity transport. It is described by the following equation[7]:

$$\frac{\partial c}{\partial t} + u\frac{\partial c}{\partial x} + v\frac{\partial c}{\partial y} + (w - w_c)\frac{\partial c}{\partial z} = \Delta_c c + f(\mathbf{x}, t) \quad (1)$$

with the initial and boundary conditions

$$c(\mathbf{x},0) = c^0(\mathbf{x}), \quad t = 0,$$
$$\frac{\partial c}{\partial x} = 0, \ \ x = 0, X, \ \ \frac{\partial c}{\partial y} = 0, \ \ y = 0, Y, \ \ \frac{\partial c}{\partial z} = 0, \ \ z = H, \quad (2)$$
$$\nu_c \frac{\partial c}{\partial z} = (\beta_c - w_c)c - f_0(x, y, t), \quad z = \delta(x, y),$$

where $c(\mathbf{x}, t)$ is the impurity concentration, t is the time, $\mathbf{x} = (x, y, z)$ are the Cartesian coordinates; $\mathbf{u} = (u, v, w)$ is the velocity of air mass, w_c is the rate of impurity sedimentation, ν_c is the turbulence factor, β_c characterizes the interaction of the impurity with an underlying surface; f and f_0 are the source functions; $\delta(x, y)$ is the function describing the relief, $c^0(\mathbf{x})$ is the field of the initial impurity concentration.

The input parameters of the problem (1) and (2) are meteoparameters (vector of wind velocity, turbulence factor, etc.) calculated by means of mesoscale non-hydrostatic model of atmosphere dynamics[7,8]:

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$$\frac{\partial \rho u}{\partial t} + \mathrm{div}\rho u\mathbf{u} = -\frac{\partial p'}{\partial x} + l\rho v + \Delta_u u,$$
$$\frac{\partial \rho v}{\partial t} + \mathrm{div}\rho v\mathbf{u} = -\frac{\partial p'}{\partial y} - l\rho u + \Delta_v v, \quad (3)$$
$$\frac{\partial \rho w}{\partial t} + \mathrm{div}\rho w\mathbf{u} = -\frac{\partial p'}{\partial z} + \lambda\rho\vartheta' + \Delta_w w,$$
$$\frac{\partial \rho\vartheta'}{\partial t} + \mathrm{div}\rho\vartheta'\mathbf{u} = -S\rho w + \Delta_\theta\vartheta', \ \ \mathrm{div}\rho\mathbf{u} = 0.$$

Here ϑ' and p' are the deviations of the potential temperature and air pressure from their reference values; $\rho = \rho(z)$ is the preset function of air density; l is the Coriolis parameter; S and λ are the stratification and buoyancy parameters. The functional Δ_α ($\alpha = u, v, w, \vartheta, c$) has the form

$$\Delta_\alpha = \frac{\partial}{\partial x}\mu_{\alpha x}\frac{\partial}{\partial x} + \frac{\partial}{\partial y}\mu_{\alpha y}\frac{\partial}{\partial y} + \frac{\partial}{\partial z}\mu_{\alpha z}\frac{\partial}{\partial z},$$

where $\mu_{\alpha x}$, $\mu_{\alpha y}$, $\mu_{\alpha z}$ are the coefficients of turbulent diffusion along x, y, and z coordinates, respectively.

The boundary conditions for Eq. (3) are formulated as follows. Homogeneous Neumann conditions are set on the side boundaries of the domain; damping of disturbances of meteoparameters is assumed at the top boundary. The influence of orographical and thermal inhomogeneities of underlying surface is accounted in the thermal balance equation on the surface and in the edge conditions on the calculated bottom level of the model, which coincides with the upper boundary of the surface layer. Application of the surface-layer theory results in the conditions of the third kind. Thus, equations of the atmospheric dynamics and transport model (1) and (2) are integrated within the domain

$$D_t = D[0, T],$$

where

$$D = \{0 \le x \le X, 0 \le y \le Y, \delta(x, y) + h \le z \le H\}, \ \ 0 \le t \le T$$

is the time slice, and h is the height of the surface layer. Ideas of the method of dummy domains are used to account for the relief. References 7 and 8 describe model (3) in a more detail. The problem of impurity transport (1), (2) is solved using the wind velocity fields obtained.

2. Models of atmospheric transport of impurities

To solve thus stated problem (1) and (2), two 3D models were used: deterministic model in Euler[7,8] formulation and deterministic-stochastic one in terms of Lagrange approach.[4–6] The gridless structure of the Lagrange model is referred to the grid structure in Euler models, using for forming hydrodynamic processes in a carrier medium.

2.1. Scheme of implementation of the Euler impurity transport model

Since the impurity concentration cannot be negative in a physical sense, finite-difference schemes having monotonicity property are of great importance in implementations of numerical models based on the transport equation with turbulent diffusion. In this study, a numerical algorithm for the 4D impurity transport model (1), (2) is constructed by means of approximation of the integral identity within the variational formulation of the model. Here analytical solutions of the local conjugate problems within the limits of three-point patterns for each of the coordinate directions[9] are used as the weighting coefficients. The variational principle was used along with the split method: the initial many-dimensional problem at each time step was approximated by an array of sequentially solved one-dimensional tasks.

To construct discrete approximations, let us introduce the grid domain D_t^h into D_t as the Cartesian product of one-dimensional grids along t, x, y, and z. In approximating, the functions u, v, w, μ_{cx}, μ_{cy}, and ν_c we assumed these functions to be step-wise constant within the grid cells

$$\Delta D_{imk} = \{x_i \le x \le x_{i+1}, y_m \le y \le y_{m+1}, z_k \le z \le z_{k+1}\} \in D_t^h .$$

Let us write the problem (1), (2) in the operator form and associate it with the discrete analog of the integral identity

$$I^h(c, c^*) =$$
$$= \sum_{j=0}^{J}\left\{\int_{t_j}^{t_{j+1}}\left(\frac{\partial c}{\partial t}, c^*\right)^h \mathrm{d}t + \int_{t_j}^{t_{j+1}}(Lc, c^*)^h \mathrm{d}t - \int_{t_j}^{t_{j+1}}(f, c^*)^h \mathrm{d}t\right\} = 0, \quad (4)$$

where

$$Lc = u\frac{\partial c}{\partial x} + v\frac{\partial c}{\partial y} + \tilde{w}\frac{\partial c}{\partial z} - \left(\frac{\partial}{\partial x}\mu_{cx}\frac{\partial c}{\partial x} + \frac{\partial}{\partial y}\mu_{cy}\frac{\partial c}{\partial y} + \frac{\partial}{\partial z}\nu_c\frac{\partial c}{\partial z}\right);$$

$\tilde{w} = w - w_c$; c^* is an arbitrary sufficiently smooth function; the superscript h marks the analogs of the corresponding expressions.

Transform Eq. (4) with the partial integration operations choosing the function c^* in the form of product of solutions of one-dimensional conjugate tasks defined on the family of cells of the grid domain D_t^h, like in Ref. 9:

$$c_{imk}^*(\mathbf{x}) = c_{imk}^* c_{x_i}^*(x) c_{y_m}^*(y) c_{z_k}^*(z).$$

Choose each of $c_s^*(s), (s = x, y, z)$ from the totality of fundamental solutions of one-dimensional equations within the cells of the grid domain along the coordinate curves:

$$L_s^* c_s^*(s) \equiv \frac{\partial}{\partial s}\rho\mu_{cs}\frac{\partial c_s^*(s)}{\partial s} + \rho u_s \frac{\partial c_s^*(s)}{\partial s} = 0,$$

$$u_s = u, v, \tilde{w}, \quad \mu_{cs} = \mu_{cx}, \mu_{cy}, \nu_c, \tag{5}$$

$$c_s^*(s_\alpha) = 1, \; c_s^*(s_{\alpha+1}) = 0; \; c_s^*(s_\alpha) = 0, \; c_s^*(s_{\alpha+1}) = 1,$$

$$s \in [s_\alpha, s_{\alpha+1}], \; \alpha = i, j, k.$$

Using the obtained functions c^*, fulfill all the integration operations in Eq. (4) and time quantization. Finally, calculate the derivatives $\partial I^{h\tau}(c_{imk}^j, c_{imk}^{*j})/\partial c_{imk}^{*j} = 0$ for all j, i, m, and k, enumerating D_t^h grid nodes, and come to the split scheme written in the form of sets of difference equations for each coordinate direction, which are solved by the sweep method at each fractional time step.

Thus constructed numerical schemes for solving the impurity transport equation have properties of stability, monotonicity, and transportability. They provide nonnegativity of concentrations, fulfillment of mass balance relations, and impurity transport with the carrier medium flux.

2.2. Algorithm for impurity transport modeling in terms of Lagrange approach

The second version of numerical model for the solution of problem (1), (2) is based on the split method and is carried out within the Lagrange approach. Describe the algorithm scheme following Ref. 4. Actually, the scheme of implementation of the Lagrange transport model (LTM) of impurities has gridless spatial and time structure. The parameters of hydrodynamic background are considered to be set on the uniform grid domain $D_t^h \subset D_t$, in model (1), (2) they are functions $\mathbf{u}$, μ, etc., calculated with the use of model state function (3). Therefore, the LTM gridless structure is referred to the grid D_t^h of the Euler model of atmospheric dynamics, i.e., particles move through the grid D_t^h, coordinates and all parameters of any current point of a particle path are identified in a corresponding 4D parallelepiped of the grid domain D_t^h, which is written in the form $\Delta D_c \equiv D_{imk}^j$.

All elements of the hydrodynamic background at a current path's point, necessary for LTM, are calculated with interpolation procedures by values of corresponding fields in the vertexes of parallelepiped accompanied this point. Denote parameters of the grid D_t^h by time and spatial variables in numerical model (3) as $\{\Delta\tau, \Delta s_E, s = x, y, z\}_{imk}^j$, while time step in LTM by Δt. To construct a numerical modeling scheme for paths of individual particles and their ensembles, the initial problem is split into three physical processes: impurity emission, transport along the path of an air mass, and turbulent exchange.

Advective transport. At the first stage, the concentration of impurities in local areas adjacent to source points is calculated. At the stage of transport deterministic elements of impurity particles paths are calculated by the preset field of velocities. Write the equation of transport along the air mass paths:

$$\frac{\partial\varphi}{\partial t} + u\frac{\partial\varphi}{\partial x} + v\frac{\partial\varphi_1}{\partial y} + \tilde{w}\frac{\partial\varphi}{\partial z} = 0, \quad t_j \le t \le t_{j+1}. \tag{6}$$

From this equation, come to the set of three equation[10]:

$$\frac{\mathrm{d}x}{\mathrm{d}t} = u(\mathbf{x}, t), \; \frac{\mathrm{d}y}{\mathrm{d}t} = v(\mathbf{x}, t), \; \frac{\mathrm{d}z}{\mathrm{d}t} = \tilde{w}(\mathbf{x}, t), \tag{7}$$

which allows calculating the particle position at each time step t_{j+1} at the preset coordinate values $\mathbf{x}^j = (x, y, z)^j$ at the time point t_j.

To construct the numerical scheme we used the approximation of the second order of accuracy:

$$\Delta x^{j+1} = u(\mathbf{x}^j, t^j)\Delta t + \frac{1}{2}(\frac{\partial u}{\partial x}\Delta x^{j+1} + \frac{\partial u}{\partial y}\Delta y^{j+1} + \frac{\partial u}{\partial z}\Delta z^{j+1})\Delta t,$$

$$\Delta y^{j+1} = v(\mathbf{x}^j, t^j)\Delta t + \frac{1}{2}(\frac{\partial v}{\partial x}\Delta x^{j+1} + \frac{\partial v}{\partial y}\Delta y^{j+1} + \frac{\partial v}{\partial z}\Delta z^{j+1})\Delta t,$$

$$\Delta z^{j+1} = \tilde{w}(\mathbf{x}^j, t^j)\Delta t + \frac{1}{2}(\frac{\partial \tilde{w}}{\partial x}\Delta x^{j+1} + \frac{\partial \tilde{w}}{\partial y}\Delta y^{j+1} + \frac{\partial \tilde{w}}{\partial z}\Delta z^{j+1})\Delta t. \tag{8}$$

The parameters of the scheme are chosen adaptive to the process intensity from the approximation and stability conditions:

$$\left(\frac{2\mu_s}{\Delta s_E^2} + \frac{|u_s|}{\Delta s_E}\right)\Delta\tau_s \le 1, \; \Delta t \le \min_{<s>}\{\Delta\tau_s\}, \; s = x, y, z, \tag{9}$$

where Δs_E are the parameters of the grid D_t^h within the parallelepiped ΔD_c accompanied a particle, $\Delta\tau_s$ is the time step at which the Courant, Friedrichs, and Levy[11] approximation conditions for the variable s are fulfilled within the subdomain ΔD_c; $u_s \equiv \{u, v, \tilde{w}\}$ are the values of velocity components; μ_s are the values of turbulence factors at the path point $(\mathbf{x}^j, t^j)$, calculated with the field of meteorological values at the vertexes of ΔD_c. Derivatives in Eq. (8) are also calculated by difference relations within the same parallelepiped.

Solving the set of equations (8) relative to $\Delta\mathbf{x} = (\Delta x, \Delta y, \Delta z)$, obtain the particle coordinates $\mathbf{x}^{j+1/2}$ at the first splitting stage (6), (7):

$$\mathbf{x}^{j+1/2} = \mathbf{x}^j + \Delta\mathbf{x}^{j+1}. \tag{10}$$

Turbulent exchange. Turbulent movement of particles at each time step is considered as a stochastic process. To construct the calculation algorithm for this process we used the method of local approximations.[12,13] Such an approach allows the complex process with inhomogeneous anisotropic turbulence to be described with the superposition of local normal random processes along the coordinate directions, the variances scale of which is calculated via the turbulence factor.

At this splitting stage, we have the following equation:

$$\frac{\partial\varphi}{\partial t}-\frac{\partial}{\partial x}\mu_x\frac{\partial\varphi}{\partial x}-\frac{\partial}{\partial y}\mu_y\frac{\partial\varphi}{\partial y}-\frac{\partial}{\partial z}\mu_z\frac{\partial\varphi}{\partial z}=0,\quad t_j\le t\le t_{j+1}. \quad (11)$$

The operator of the turbulent exchange model in Eq. (11) with variable coefficients within the method of local approximations is substituted for a the set of operators with piecewise-constant coefficients on the principle of "frozen coefficients."[12,13] Here the locality is regarded in the space of turbulence factor values. At such assumptions, each local-relative-to-μ_s Eq. (11) has constant coefficients and allows variables separation. At every time step $t_j \le t \le t_{j+1} = t_j + \Delta t$ the 3D problem is approximated to the set of three one-dimensional analytically solvable problems.

Taking this into account as well as the correlations between ND probability-density functions and Green functions for the set of diffusion equations, model the turbulent process of particles dispersal as the superposition of Gaussian random processes in the neighborhood of path point coordinates [Eq. (10)]. For every point we used its own coefficient μ_s. The step value of Δt is chosen adaptive to local conditions in the neighborhood of point $\mathbf{x}^{j+1/2}$ from Eq. (10) according to Eq. (9). In ensemble calculating the algorithm parameters are adjusted for every particle separately.

Owing to such modeling, the increments of particle coordinates at the stage of turbulent mixing are calculated as follows:

$$\zeta_x = q\sqrt{2\mu_x\Delta t},\quad \zeta_y = q\sqrt{2\mu_y\Delta t},\quad \zeta_z = q\sqrt{2\mu_z\Delta t}, \quad (12)$$

where q are the normally distributed random variables with zero mean and unit variance. Final equations for the particle coordinates are

$$\mathbf{x}^{j+1} = \mathbf{x}^{j+1/2} + \xi,\quad \xi \equiv (\xi_x,\xi_y,\xi_z). \quad (13)$$

The path of every particle is calculated till "control" time or particle ingress to the receptor domain, or running out of the domain.

Edge conditions (2) in LTM are taken into account in the following way. At the bottom and side boundaries of the domain ΔD_c, when the particle coordinates, calculated by Eqs. (8), (10) and (12), (13), turn out to be out of the domain, the particle is regarded as ceasing to be and its contribution is taken into account when estimating impurity flows over the border. At the bottom boundary of the domain D_t in the model is specified a mixed edge condition to take it into account, specific modifications are introduced into the scheme to describe particle motion in the surface layer with the account for underlying surface irregularities, temperature stratification, and the probability of surface deposition. The parameterized effective bottom boundary of an air mass is determined from such a modification. A particle moves until it passes through this border.

3. Numerical experiments

To compare the calculated results, a series of experiments was carried out on simulating the transport of a passive impurity in a mountain-and-valley region based on the models used. The region for which the fields of meteoelements were obtained by model of atmospheric hydrodynamics (3), which are required for calculating impurity transport by model (1), (2), is a valley elongated from southwest to northeast. The relief causes diurnal variations of wind direction and strength in the region. A source of passive impurity is located in the valley's center. Modeling was carried out for summer period.

Three time intervals of 3 hours were chosen for the calculations. A situation corresponding to the morning circulation development was considered in the first experiment. The second one reflects the specific of impurity transport in daylight while the third one – in the evening. For all scenarios we specified the following values of input parameters: domain sizes $\{X = 50$ km, $Y = 48$ km, $H = 2.5$ km$\}$, steps of the grid domain $\{\Delta x = \Delta y = 2000$ m, $\Delta z_k = 100$ m$\}$, "basic" time step in the Euler model $\Delta\tau = 10$ s, turbulent diffusion coefficients $\mu_{cx} = \mu_{cy}$ calculated by the Smagorinskii model, vertical coefficient $\nu_c = 3$ m^2/s. An emission source was regarded as instantaneous, with the coordinates $\{x = 28$ km, $y = 24$ km, $z = 100$ m$\}$. The impurity was considered as weightless, i.e., $w_c = 0$ m/s. When calculating by the model of Lagrange type, action of the source was specified an instantaneous emission of 1000 particles.

For the chosen calculation domain, summer morning circulation is characterized by attenuation of katabatic winds developed in nighttime, weak wind along the valley, and formation of ascending currents. Figure 1 shows the fragment of the vertical section of wind field and impurity concentration at $x = 28$ km.

The results calculated by the Euler model are shown in Fig. 1*a* while Fig. 1*b* corresponds to the Lagrange one. Isolines in Fig. 1*a* show the impurity concentration in fractions of 1000 in 1 hour after the emission. Dots in Fig. 1*b* represent impurity particles. As the motion is three-dimensional, then the vertical section represents only a part of its complicated structure. Movement of impurity particles in a circulation cell, formed by air currents ascending from the bottom and katabatic winds, is well seen in Fig. 1*b*.

Similar sections of fields of impurity concentration and wind for daylight and evening time in 1 hour after the emission are shown in Figs. 2 and 3. Daytime circulation is characterized by ascending currents along heated hangs and weak movement of air mass in the valley. In the evening, the southeast hang begins to cool first, which results in the formation of air currents from the cooler hang to the warmer one.

The comparison shows qualitative agreement of model results on impurity transport for both models. The pollutant cloud moves downwind in all cases. More fuzziness of pictures, obtained in Euler approach, is explained by relatively wide domain of influence of the resolving operator of implicit scheme, even under conditions (9). This manifests itself in the effects of solution smoothing. To weaken them, the resolution of discrete schemes is to be enhanced. The work within subgrid scales is possible in Lagrange approach under conditions (9) and, hence, a detailed presentation of development of the processes is obtainable.

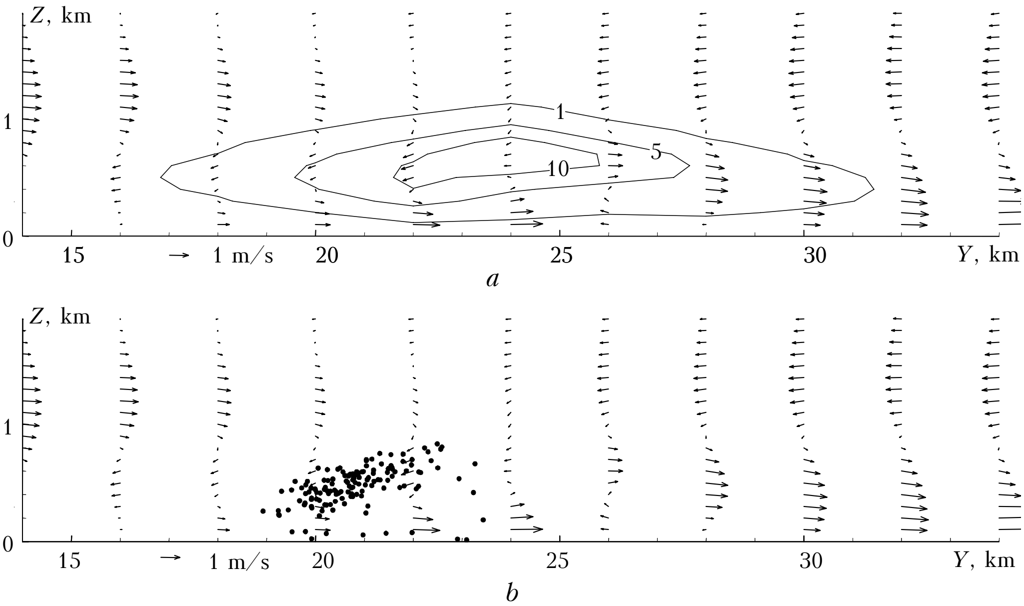


Fig. 1. Vertical sections of the fields of wind and impurity concentration at $x = 28$ km in 1 hour after the emission: Euler (*a*) and Lagrange (*b*) models. Morning circulation.

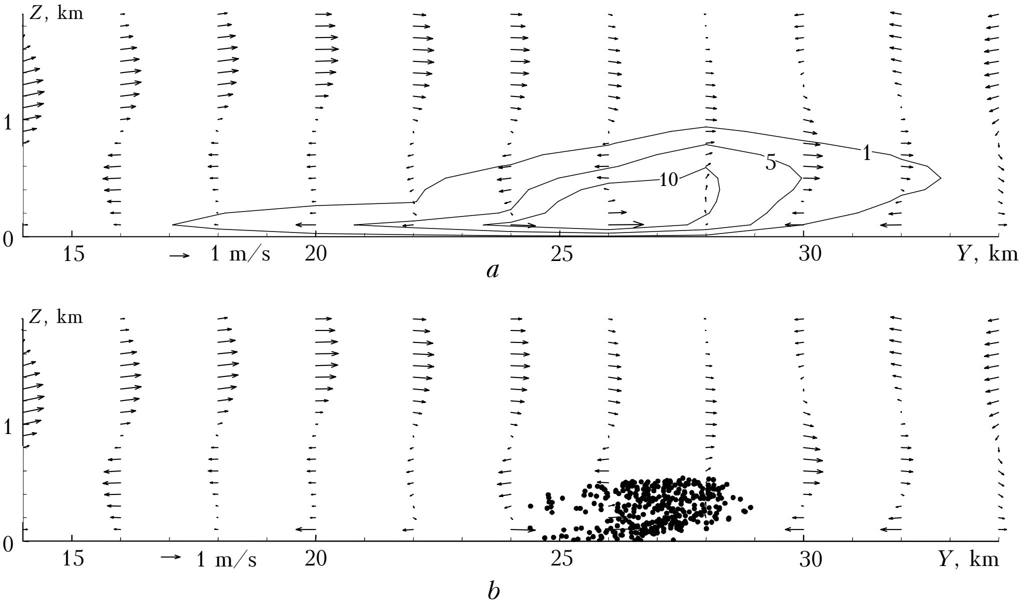
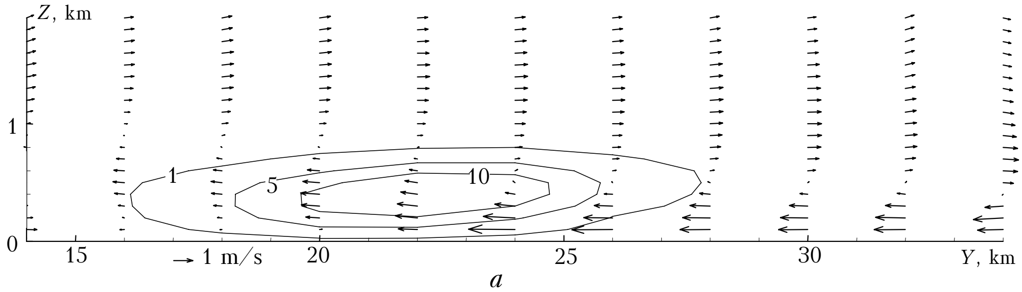


Fig. 2. Similar to Fig. 1, daytime circulation.



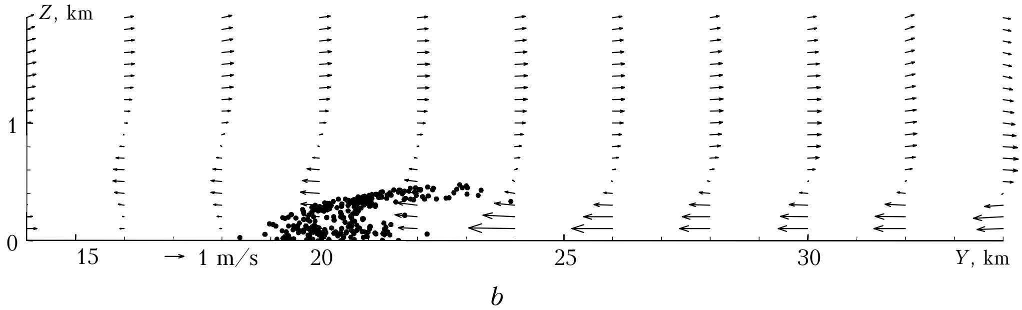


Fig. 3. Similar to Fig. 1, evening circulation.

Conclusion

The algorithms have been described for implementation of the models of atmospheric transport of impurities in Euler and Lagrange terms, developed at ISM&MG SB RAS.

The modifications of numerical impurity transport models used are realized as a set of routines, agreed on the level of data arrays and adapted for the work with models of the fields of hydrometeorological elements generation in the atmosphere.

The analysis of modeling scenarios showed similar results from both approaches. As for specificity of implementation, algorithms of both models require adaptation to the intensity of processes. Work of Euler model is traditional for such kind of models, it represents general nature of processes within the whole domain. The model of Lagrange type is easier controllable in tracking of processes intensity. Its calculating core is easy adaptable, this allows the model to be linked, e.g., in cases when more detailed representation of development of processes is required in characteristic local zones and regions, adjoining to sources of emission and runoff of impurities.

Thus, both model versions complement each other and can be used for forecast and diagnosis purposes when studying nature.

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