

Modeling of processes of pollutant transport in direct and inverse problems of climato-ecological monitoring and prediction

V.V. Penenko and E.A. Tsvetova

*Institute of Computational Mathematics and Mathematical Geophysics,
Siberian Branch of the Russian Academy of Sciences, Novosibirsk*

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A new version of a set of mathematical models for investigating transport and transformation of pollutants from natural and anthropogenic sources in the atmosphere is presented. The structure of the models, methods of discretization, and algorithms realizing the various models are constructed for application to direct and inverse modeling in problems of monitoring, forecasting, and ecological planning. Toward this end, a variational principle in combination with decomposition and splitting techniques is used to construct the numerical models. Algorithms for calculating the direct and adjoint trajectories in the source-detector system are described. Examples are given of solutions of the direct and inverse problems for estimating the scales of interactions of the type (source) – (conservation zone) (Lake Baikal).

Processes of transport and transformation of pollutants from natural and anthropogenic sources have become an important factor in the climatic system of large cities and industrial regions. Their description and forecasting require mathematical models adequately reflecting hydrometeorological and ecological situations in real time and over extended periods.

At present, efforts in the direction of air-quality control in Russia and elsewhere make wide use of models, which can nominally be called models for “simultaneous” control of air quality. These are various modifications of models of Gaussian type and are based on solutions of steady-state equations of pollutant transport in simplified formulations. In Russia, models of such type are certified at a high administrative level and are recommended as the official methodology for use in the development of conservation measures and to realize government control of air quality.¹ The principal advantage of models of the given class over complex numerical models consists in their simplicity and economy of realization in a probabilistic description of the process of the spreading of a pollutant under uniform steady-state conditions. Nowadays they have been adapted for autonomous use on a personal computer and in the context of local geo-information systems (GIS) are in active use throughout Russia and the CIS.

It should be borne in mind that in all cities of the CIS, the air-quality conservation measures in use implement this official methodology. Therefore, every active industrial entity and every new project that may have an effect on the environment acquire a right to exist only after it has been determined that they meet the requirements of maximum permissible emissions (MPE) of pollutants on the basis of this official

methodology. An analysis of the air-quality of cities of the CIS during the last 20 years shows that the majority of them find themselves in a state which, according to many indices, is far from ecologically favorable. Hence we may conclude that the official methodology in use today is not fully suited for dealing with the problems of forecasting air-quality under actual conditions. It is necessary to develop new approaches to the solution of ecological problems and for estimating the efficiency of conservation measures. In the near future such efforts will become extraordinarily urgent for the following reasons:

- in Russia a global orientation is currently underway toward the development of raw-material related industries; a tendency is also noted toward the creation of high-output power plants with the goal of the production of energy for export;

- on the other hand, the worldwide community has come to various decisions regarding the introduction of international quotas on the volume of emissions. This requires the imposition of controls on transboundary transport of pollutants;

- according to predictions of the Russian Ministry of Emergency, in the near future this country can expect an increase in the number of technogenic catastrophes, and these predictions are in accord with the conclusions of the European Economic Commission of the UN (Ref. 2);

- the risk of large-scale military operations of the type “Desert Storm” has increased, the consequences of the occurrence of which as a result of atmospheric transport would have a global character.

With such perspectives, ecology rises to the level of a strategic and essential socio-economic factor in the context of public policy.

1. Model of transport and transformation of pollutants

For convenience in the construction of the numerical schemes and algorithms realizing them for direct and conjugate problems, we will use a double description of the models: (1) in the form of a system of differential equations of transport and transformation of multicomponent pollutants and (2) in the form of a variational formulation employing the integral identity.

The basic system of equations of the model is written as

$$(\Lambda\varphi)_i \equiv \frac{\partial \pi \varphi_i}{\partial t} + L(\pi \varphi_i) + B(\varphi)_i = f_i, \quad (1)$$

$$i = \overline{1, n}, n \geq 1.$$

Here $\varphi = \{\varphi_i(\mathbf{x}, t), i = \overline{1, n}\} \in Q(D_t)$ is the state-function vector; φ_i is the concentration of the i th pollutant; n is number of different substances, $\mathbf{f} = \{f_i(\mathbf{x}, t), i = \overline{1, n}\}$ are the source functions, $L(\mathbf{x}, t)$ is the advection-diffusion operator, $B(\varphi)$ is the pollutant transformation operator; π is a function of the pressure, whose form depends on the choice of the coordinate system; $D_t = D \times [0, \bar{t}]$; D is the domain of variation of the spatial coordinates \mathbf{x} , and $[0, \bar{t}]$ is the time interval; $Q(D_t)$ is the space of state functions satisfying the boundary conditions on the boundary of the domain D_t . If the presence of errors is assumed in the model, then expressions describing them are formally included in the source functions as additional terms.

A constructive description of the pollutant transformation operators is achieved with the help of an automated system for constructing kinetic models of atmospheric chemistry.^{3,4}

The variational formulation of the model has the form

$$I(\varphi, \varphi^*, \mathbf{Y}) \equiv \int_{D_t} (\Lambda\varphi - \mathbf{f})\varphi^* dDdt = 0, \quad (2)$$

where $\varphi^* \in Q^*(D_t)$ is a function with sufficiently smooth components; $Q^*(D_t)$ is the function space conjugate to $Q(D_t)$; $\mathbf{Y} = \{Y_i, i = \overline{1, n}\} \in R(D_t)$ is the parameter vector of the model; $R(D_t)$ is the domain of accessible values.

For problems of monitoring, forecasting, planning and control, and to organize the inverse modeling algorithms, we introduce the set of functionals

$$\Phi_k(\varphi) = \int F_k(\varphi)\chi_k(\mathbf{x}, t) dDdt, k = \overline{1, K}, K \geq 1, \quad (3)$$

where $F_k(\varphi)$ are prescribed functions on the set of state functions, differentiable with respect to φ ; $\chi_k \geq 0$ are the weight functions, and $\chi_k dDdt$ is a Radon or Dirac measure in D_t .

Three variants of the domain D are considered: a sphere, a hemisphere, and a bounded region on the sphere. The structure of the domains, choice of coordinate system, basic notation and its meaning, statement of the boundary conditions and initial conditions, a description of the state functions and parameters, the structure of the functionals as a function of the purpose of the study, and the method of constructing the integral identity are all described in Refs. 5-8.

The numerical schemes and the algorithms realizing the models are constructed using the variational principle in combination with splitting and decomposition methods. The integral identity (2) is used to achieve this end. In the splitting method the main discretization element of the model is constructed on the basis of relations of the form⁹

$$\int_{x_{\alpha-1}}^{x_\alpha} (\Lambda_x \varphi - f)\varphi^* dx =$$

$$= \int_{x_{\alpha-1}}^{x_\alpha} \Lambda_x^* \varphi^* \varphi dx - (A_x \varphi, \varphi^*) \Big|_{x_{\alpha-1}}^{x_\alpha} - \int_{x_{\alpha-1}}^{x_\alpha} f \varphi^* dx, \quad (4)$$

where φ is one of the components of φ , x is one of the spatial coordinates, Λ_x is that part of the operator Λ , in the context of the splitting method, operating in the x direction; $[x_{\alpha-1}, x_\alpha]$ is the α th grid cell in x ; $\alpha = \overline{1, M}$; Λ_x^* is the operator conjugate to Λ_x ; $(A_x \varphi, \varphi^*)$ are relations at the boundaries of the cells in x , and the form of the operator A_x is determined by the structure of the operator Λ_x .

How the model is discretized depends on how the functions φ^* are assigned in Eq. (4). For example, for $\varphi^* = \text{const}$ for advection-diffusion problems we obtain schemes of the integral-interpolation balance method. We choose the functions φ^* such that they are solutions of the local conjugate problems

$$\Lambda_x^* \varphi^* = 0, x_{\alpha-1} \leq x \leq x_\alpha, \alpha = \overline{1, M}. \quad (5)$$

These solutions, given the corresponding assumptions regarding approximation of the coefficients of the operator Λ_x within the limits of the grid cells, are found analytically and then substituted into Eq. (4). Examples of the use of this discretization method are described in detail in Ref. 9. Finally, its application leads to numerical schemes of variational-difference type.

To approximate the integral identity (2) in time, we use the method of weak approximation with fractional time steps.⁵ In this method, the pollutant

transformation operators are taken into account at each fractional step. As a result of the discretization, we obtain the discrete analog of the integral identity

$$I^h(\varphi, \varphi^*, \mathbf{Y}) = 0, \quad (6)$$

$$\varphi \in Q^h(D_t^h), \quad \varphi^* \in Q^{*h}(D_t^h), \quad \mathbf{Y} \in R^h(D_t^h).$$

Here the superscript h denotes the discrete analog of the corresponding objects. In the grid domain D_t^h we also construct the discrete analogs of the functionals $\Phi_k^h(\varphi)$ [Eq. (3)]. Here it is essential that the discretization of the integrals and state functions in identity (6) and in the functionals (3) be performed on the same grid so as not to introduce additional transformation operations from one grid to the other. In the decomposition of the domain D into subdomains, this alignment should be maintained even though the grids in the subdomains can be introduced differently.

The numerical schemes and algorithms are obtained from the conditions:

for the direct problem

$$\frac{\partial I^h(\varphi, \varphi^*, \mathbf{Y})}{\partial \varphi^*} = 0, \text{ for all } \varphi^* \in Q^{*h}(D_t^h), \quad (7)$$

for the conjugate problems

$$\frac{\partial I^h(\varphi, \varphi_k^*, \mathbf{Y})}{\partial \varphi} + \frac{\partial \Phi_k^h}{\partial \varphi} = 0, \text{ for all } \varphi \in Q^h(D_t^h), \quad (8)$$

$$\varphi_k^*(\mathbf{x}, \bar{t}) = 0; \quad k = \overline{1, K}.$$

The sensitivity relations for the functionals

$$\begin{aligned} \Phi_k^h(\varphi) &\equiv (\text{grad}_{\mathbf{Y}} \Phi_k^h(\varphi), \delta \mathbf{Y}) = \\ &= \frac{\partial}{\partial \xi} I^h(\varphi, \varphi_k^*, \mathbf{Y} + \xi \delta \mathbf{Y}) \Big|_{\xi=0}, \quad (9) \\ &k = \overline{1, K}, \end{aligned}$$

where the symbol δ denotes variation of the corresponding quantities, ξ is a real parameter, $\delta \mathbf{Y} = \{\delta Y_i, i = \overline{1, n}\}$ is the vector of variations of the parameters \mathbf{Y} , $\text{grad}_{\mathbf{Y}} \Phi_k^h(\varphi) \equiv \Gamma_k$ are the sensitivity functions of the functional with index k to variations of the parameter vector. Their explicit form is obtained by equating the coefficients on the left and right-hand sides of Eq. (9) for the corresponding components of the vector of variations of the parameters or directly by differentiating the expression in discrete form for the functional

$$\Gamma_{ki} = \frac{\partial}{\partial Y_i} I^h(\varphi, \varphi_k^*, \mathbf{Y}), \quad k = \overline{1, K}, \quad i = \overline{1, N} \quad (10)$$

for all $\mathbf{Y} \in R^h(D_t^h)$ for prescribed φ and φ_k^* .

Since we used the method of weak approximation with fractional steps and decomposition of the domain

D into subdomains in the approximation of the integral identity (2), the systems of basic equations (7) and conjugation equations (8) are splitting schemes decomposed into subdomains. The method of their construction with the help of Eq. (6) ensures mutual alignment of these schemes. Their specifics are such that the transport processes are approximated for each species individually, but over the entire domain D_t^h . The pollutant transformation processes are described by a set of chemical-kinetic "point" models for the entire set of species at each point of the grid independent of the other points.⁴

It should be noted that the conjugate functions in the method are employed in two different senses. First, in the local sense, as solutions of the sets of local conjugate problems (5), which are chosen as weight functions in the construction of the discrete analogs of the operators in identity (6). And, second, in the global sense, as solutions of the global conjugate problems (8) linking the functions with the model (1). They are also used to obtain the sensitivity relations (9) and the sensitivity functions (10).

We may make one more remark regarding the organization of the modeling process. In optimization problems of ecological planning, when it is necessary to calculate many different scenarios it is troublesome to work with time-dependent transport models: the large number of internal degrees of freedom requires a correspondingly large amount of calculation to reach steady state. Therefore, in those cases when the temporal variability of the processes has large characteristic scales it makes sense to consider scenarios that have already reached steady state, i.e., to solve steady-state problems. This can substantially reduce the amount of work and give a good first approximation for further study.

Under these assumptions, the time derivatives in model (1), Eq. (2) can be dropped. The discretization procedure based on the integral identity (2) and the structure of the algorithms remain the same, only in this case, the spatial variable that enters as the "marching" variable—the variable in which splitting of the problem and the dynamics of the modeled processes are realized—is the spatial variable in which the predominant motion of the flux of air masses occurs.

In the construction of the numerical schemes for the transport model the hydrothermodynamic components of the state function of the atmosphere are assumed to be known. They can be assigned in various ways. In particular, they can be calculated from models of the dynamics of the atmosphere functioning in combination with the transport models.

2. Algorithms for calculating particle trajectories

The modeling methods considered above are based on an Eulerian description of advection–diffusion

processes of material transport. In practice, one frequently encounters the need to calculate the spreading of pollutants in moving volumes of air masses, i.e., using the Lagrangian approach. These approaches are not alternative approaches, rather they complement each other. Each of them has its own advantages and shortcomings, and its own region of applicability.¹⁰

Here we will describe the basic elements of the algorithm of “non-grid” modeling of the trajectories of the pollutant particles under the assumption that the hydrometeorological parameter fields of the atmosphere are given on some grid D_t^h in D_t . In accordance with the definition of direct and inverse modeling, we construct the algorithms for calculating the direct and conjugate (inverse) trajectories.

We construct the structure of the numerical schemes using the method of splitting over physical processes. In the domain D_t^h over sufficiently short intervals of time of length Δt we define two splitting steps:

- 1) transport over trajectories of air masses

$$\frac{d\phi}{dt} = 0; \tag{11}$$

- 2) turbulent exchange

$$\frac{\partial \phi}{\partial t} - \text{div} \mu \text{grad} \phi = 0, \tag{12}$$

where $\mu = (\mu_1, \mu_2, \mu_3)$, $\mu_i (i = \overline{1,3})$ are the coefficients of turbulent exchange in the x_i directions ($i = \overline{1,3}$). The direct trajectories are modeled in the direction of increasing time, and the inverse trajectories, in the direction of decreasing time.

In contrast to the Eulerian approach, splitting in the Lagrangian approach is realized along the particle trajectories. In the first step (11) the solution consists of integrating the system of equations

$$\frac{dx_i}{dt} = u_i(\mathbf{x}, t), \quad i = \overline{1,3},$$

$$\mathbf{x} = (x_1, x_2, x_3) \in D, \quad t_j \leq t \leq t_{j+1}, \tag{13}$$

where $u_i(\mathbf{x}, t)$ are the velocities of transport in the x_i direction, and u_3 takes into account the velocity of gravitational settling of the particles.

To construct the second step (12), we use the local approximation of the operator of the type “frozen” coefficients.¹¹ In this approach, for each trajectory one constructs a family of local approximations of problem (12) with constant coefficients in the domain D_t , which, however, are parametrically dependent on the coordinates of the current point of the trajectory. In other words, the constant coefficients of the local problem are equal to the values of the coefficients of problem (12) at the indicated point of the trajectory.

Under such assumptions, each local problem admits separation of variables and, consequently, the Green’s function for it can be represented as a product of the Green’s functions for the one-dimensional equations in the separate coordinates. The Green’s function for one-dimensional equations of the type (12) is identical to the probability density of Gaussian random variables with zero mean and standard deviation $\sigma_i = \sqrt{2\Delta t \mu_i}$ ($i = \overline{1,3}$).

Omitting intermediate steps, we write out the final schemes of the algorithms:

for the direct trajectories

$$\frac{\Delta x_\alpha^j}{\Delta t} = u_\alpha^j(\mathbf{x}, t) + 0.5 \sum_{k=1}^3 \frac{\partial u_\alpha^j}{\partial x_k} \Delta x_k^j, \tag{14}$$

$$\Delta x_\alpha^j = x_\alpha^{j+1/2} - x_\alpha^j, \quad \alpha = \overline{1,3},$$

$$x_\alpha^{j+1} = x_\alpha^{j+1/2} + \eta_\alpha^{j+1/2}, \quad j = \overline{1, J-1}; \tag{15}$$

for the inverse trajectories

$$x_\alpha^{*j+1/2} = x_\alpha^{*j+1} + \eta_\alpha^{*j+1}, \quad j = \overline{J-1, 1}, \tag{16}$$

$$\frac{\Delta x_\alpha^{*j}}{\Delta t} = u_\alpha^{*j+1}(\mathbf{x}, t) + 0.5 \sum_{k=1}^3 \frac{\partial u_\alpha^{*j+1}}{\partial x_k} \Delta x_k^{*j}, \tag{17}$$

$$\Delta x_\alpha^{*j} = x_\alpha^{*j} - x_\alpha^{*j+1/2}, \quad \alpha = \overline{1,3}.$$

Here $\eta_\alpha^{j+1/2}$ and η_α^{*j+1} are the normally distributed random variables with zero mean and standard deviations $\sigma_\alpha^{j+1/2}$ and σ_α^{*j+1} in the method of local approximations for problem (12); the index j counts the time steps, J is the total number of time steps on the interval $[0, \bar{t}]$. The numerical scheme (14) and (17) approximate Eqs. (13) to second order in time.

Systems (14) and (17) are solved for the increments of the coordinates by elimination. The direct trajectories are calculated starting from the region, in which the pollutant particles are distributed at the time $t = 0$ or from the coordinates of the pollution sources.

The conjugate trajectories are modeled by trajectories emanating from the “conservation” zone or from the coordinates of the observation point at the time $t = \bar{t}$ in the direction of the initial time (backwards in time). As in the case of the solution of conjugate problems, the conjugate trajectories have only informational significance. They can be defined as the Lagrangian analog of conjugate problems in models of Eulerian transport. They give information about the prehistory of the pollutants entering into the conservation zone or into the region of an observation point.

The introduction of random characteristics into the calculational algorithm at the step at which turbulence is taken into account envisages use of the technique of statistical modeling over an ensemble of particles. If turbulent exchange is neglected, it is possible to work with individual particles to calculate their direct and conjugate trajectories.

3. Modeling scenarios of source–detector type

The set of models and basic algorithms is an open, developed system of modeling. This development is continuously stimulated by new formulations of problems of ecological monitoring, forecasting, and planning. Here we present an example of the solution of two typical problems, choosing as our pollution “source” the Chernobyl Nuclear Power Plant, and as our detector-zone (conservation zone or region of observation points)—Lake “aikal. The problems were solved for the Northern Hemisphere, and the structure of the regions, the hybrid coordinate system, and the grid regions are described in Ref. 8. The main goal of the numerical experiments was to estimate the scales of interactions of the type “source–detector.”

In order to ensure the reliability of the estimates, we used retrospective factual information about the atmospheric circulation in our calculations, obtained from the Reanalysis NCEP/NCAR database (USA) (Ref. 12) for April–May 1986. Emission of pollutants from the source was taken into account in a scenario in the time interval since April 26 till May 5, 1986, which corresponds to the period of intense emission of radionuclides. The observations functional was defined over the time interval since May 3 till May 13, 1986.

To organize the modeling scenarios according to the Reanalysis data, we regenerated the detailed spatiotemporal structure of the state functions of the atmosphere in the regimes of direct and inverse modeling in the chosen time interval. Toward these ends, we used an information model based on methods of learning and interpolation of data guided by the basic model.¹³

The first problem was solved by direct modeling. Its solution demonstrates the character of the processes of pollutant spreading from sources. For the second problem, we used the method of inverse modeling. Its solution provides information about the danger that the detector-zone will receive pollution from every source located in the spatiotemporal region of influence and about the scales of this region. It also shows by what paths this danger moves toward the detector.

Figures 1 and 2 show fragments of the direct modeling scenario. Figure 1 shows the distribution of the concentration of pollutants over the surface of the Earth on May 13, 1986. Figure 2 shows the total concentration of pollutants during the period since April 26 till May 13, 1986. The concentrations are given in relative units to obviate the need for a

discussion here of questions of interpretation of the results of the calculations at the informational level in terms of actual concentrations. We consider this calculation as a “tracer” scenario.

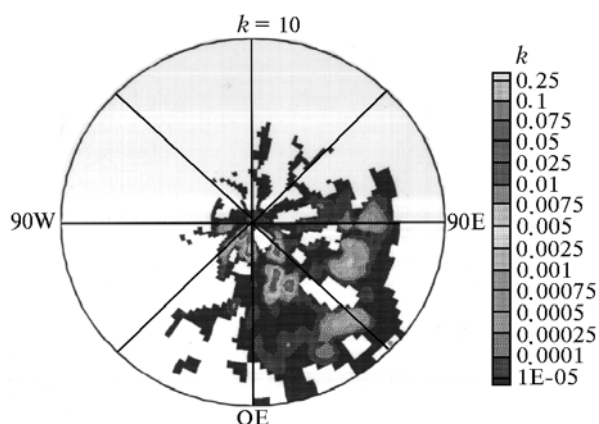


Fig. 1. Pollutant concentration k on the Earth's surface on May 13, 1986. OE denotes the Greenwich meridian.

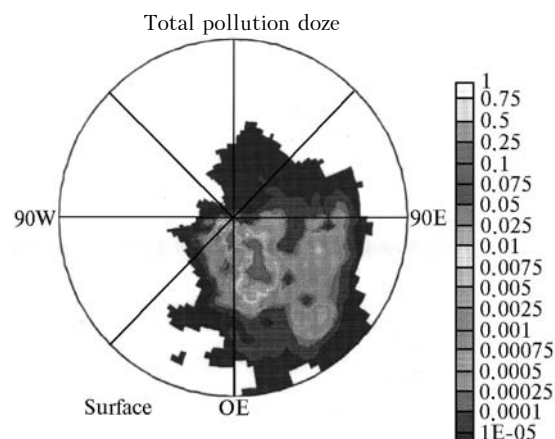


Fig. 2. Total pollutant concentration on the Earth's surface during the period since April 26 till May 13, 1986.

Figures 3 and 4 show fragments of the solution of the conjugate problem for the observation functional. According to its definition (3), this functional contains $F_k(\varphi) \equiv \varphi$, and the weight function χ_k is nonzero at the grid points that overlie Lake “aikal during the time interval since May 3 till 13, 1986. Under such conditions, the functional is an estimate of the total pollution received by the indicated region during the indicated time interval. The solution of the conjugate problem in this sense is the sensitivity function of the functional to variations of the pollution sources or the influence function of the sources for the magnitude of the estimated functional. Figure 3 presents the instantaneous value at the time 01:00, Tomsk local time on April 26, 1986 of the influence function of the sources located on the Earth's surface in the Northern Hemisphere for the magnitude of the observations

functional. Figure 4 shows the total hazard function for pollution of Lake "aikal by sources in the Northern Hemisphere during the time period since April 26 till May 5, 1986, i.e., the period of intense emission from Chernobyl.

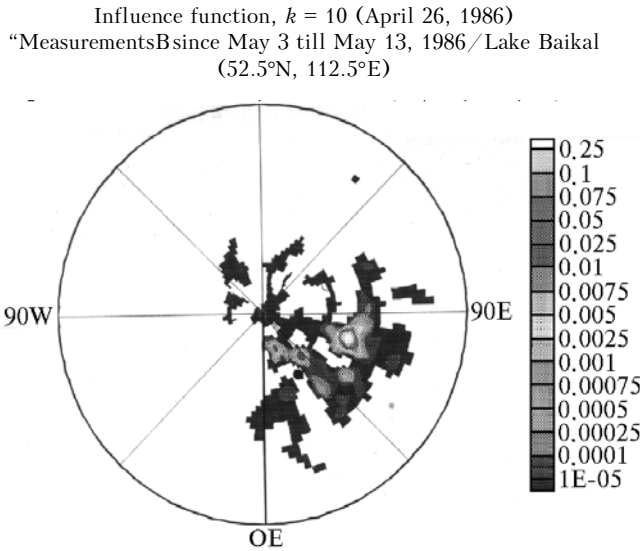


Fig. 3. Influence function at 01:00, LT on April 26, 1986 on the Earth's surface for the measurement functional during the period since May 3 till May 13, 1986.

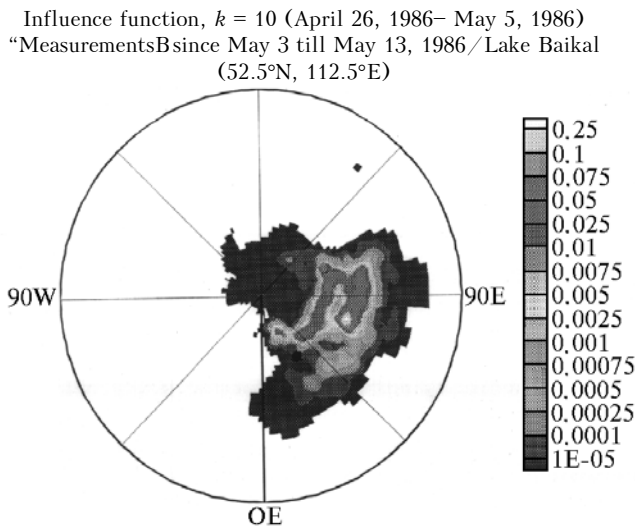


Fig. 4. "HazardBfunction for Lake Baikal during the period since April 26 till May 13, 1986 on the Earth's surface. The measurement functional during the period since May 3 till May 13, 1986.

Note the hazard function is a two-parameter function. One of these parameters is the time interval, during which the sources act, and the second is the time interval, during which measurements are taken or for which the functional is estimated. It characterizes the contribution of every source during the period it is active in the model on the value of the functional during the observation period. The influence function

and the hazard function allow one to identify the most dangerous sources, and therefore they are the most important elements in the solution of the inverse problems of estimating the strength of the pollution sources acting on the detector-zone.

An analysis of our modeling results demonstrates the global character of the processes of pollutant transport and the global character of the hazard function for pollution of a specific region. Therefore, without estimates of the hazard functions and the scales of the regions of influence of the pollution sources it would be impossible to correctly pose the problem of investigating processes of a meso-regional scale. In particular, in the scenario under consideration the pollution hazard function shows that pollution can enter the region of Lake "aikal not only from the territories of the CIS, but also from the territories of China and Mongolia. The reason for this is that starting from early May the influence of westerly-easterly transport of air masses predominates at the same time that the influence of the Sayan-Altai cyclogenesis begins to strengthen, which becomes predominant during the summer months.

4. Conclusion

The methodology of studying processes of transport and transformation of pollutants, based on principles of direct and inverse modeling using a variational approach and optimization, allows one to fully utilize the multifunctional possibilities of numerical modeling. In the first place, this pertains to the organization of the closed cycle of information processing in the system model-observations by means of the appropriate choice of criteria and functionals. In this case, a matched description of processes of different scales is ensured on the level of discrete approximations and the algorithms realizing the models.

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