Theoretical principles of the joint use of the observation data and models to study processes of hydrothermodynamics and pollutant transfer in the atmosphere

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Methodological and algorithmic aspects of combining mathematical models with the results of observations and experiments in studying real processes are discussed. The theoretical grounds for such constructions are the variation principles and the methods of optimization as applied to joint models of atmospheric hydrothermodynamics and the models of transfer and transformation of pollutants. Relations of the theory of model sensitivity and algorithms for their implementation are constructed for these combinations. The algorithms allow simultaneous estimation of relative contributions from each factor to variations of the characteristics under study, as well as evaluation of the tendencies of their influence.

Introduction

Specialists in different research areas study various aspects of mathematical support of the studies of pollutant transfer and transformation under conditions of Siberian atmosphere.[1] These studies are aimed, in particular, at gaining new knowledge about the processes under study by using jointly the mathematical models and data of laboratory and *in situ* experiments. Thus gained knowledge is targeted at the development of new approaches to solving problems in analysis and prediction.

The study of pollutant transfer and transformation in the atmosphere is of principal importance for solution of related problems of the environmental protection, ecology, and assessment of climatic changes. Among numerous disturbing factors in the Earth's system (agriculture, industrial and other human activities), changes in the chemical composition of the atmosphere are most thoroughly studied. Estimates show that the relative content and the global balance of chemically and optically active gases depend not only on numerous chemical, photochemical, and transfer processes, but also on the atmosphere–surface (waters, ocean, vegetation) exchange processes and especially on the emission and sedimentation of pollutants.

The mechanisms of secondary pollution of the environment with products of transformation of the primary pollutants are also of great importance because the products of transformation may be more active and toxic than their precursors; so they may be more hazardous to human health and the environment. A direct influence is primarily observed on local scales and mesoscales of cities and industrialized regions, where the emissions occur. This affects climatic processes indirectly through the interaction of gaseous pollutants and aerosols under the radiative processes in the atmosphere.

The climatic significance of aerosols in the atmosphere has been recently evaluated more specifically:

– the atmospheric aerosol has the tendency to produce negative radiative forcing (that is, favors cooling);

– the aerosol forcing may be significantly strong on the local scale, so that sometimes it is stronger than the positive effect (heating) due to the green house effect.

The latter conclusion can be considered as a warning of a real possibility of ecologically adverse and even catastrophic situations in the highly industrialized regions because the effects of cooling lead to accumulation of pollutants in the near-ground atmospheric layer. This increases the significance of studies of transfer and transformation of pollutants together with a study of conditions for formation of mesoclimates taking into account the competition of the urban island of heat and the green house effect with the "aerosolB cooling. Besides, this stimulates conducting specialized *in situ* experiments in order to detect these phenomena. The practical importance of these studies is in revealing prerequisites of ecological disasters and preventing them.

Structure of the data and models of observations

The function of state falls in the category of fundamental characteristics of an object or process under study and the corresponding mathematical models. However, evaluation of the actually observed behavior of a system with using only the functions of state often proves inefficient. For successful studies the direct and inverse relations between the results of observations and the mathematical model of a process or its input parameters should be known and realizable in practice.

The results of observations can be described with the function of distribution of devices in a given space–time region and a set of values of the parameters measured. Measurements can be classified as contact, remote, and indirect by their content and methods used.

Prior to the discussion of general problems on the relations between observations and models of the processes, we should first answer the fundamental and, at the same time, specific practical question: What is the mathematical expression for the results of observations in terms of the function of state, which participates in the mathematical model for description of the processes or objects under study? In other words, we should find the mathematical models for observations themselves. In the general case, it is a set of models because every type of observations and measuring or observing device has its own algorithmic presentation in terms of informative and numerical description of the components of the function of state. For example, in contact observations the values of the function of state are measured directly. If there is no measurement error, then the operator of a model of observations is simply an identical operator in such cases. In remote measurements, the model of observations is usually based on integral operators acting in space and time on the set of values of the function of state.

Let D_t denote the area, where the observed processes take place and the mathematical model describing these processes is defined. Assume that observations are realized on some set of points $D_t^m \subset D_t$, which contains at least one point. Since the numerical model on the discrete area $D_t^h \subset D_t$ is involved in calculations, the set of points D_t^m can also be considered discrete:

$$\{(\mathbf{x},\, t)_\beta,\ \beta = \overline{1, r}\ ,\ r \geq 1\} = D_t^m.$$

The set of observed values is denoted by the vector ψ^m, while the set of values calculated with the models is denoted as $[\psi]^m$:

$$\psi^m = \{\psi^m_{\alpha\beta} \equiv [H_\alpha(\varphi)]^m_\beta + [\xi_\alpha(\mathbf{x},\, t)]^m_\beta\}\ ; \tag{1}$$

$$\alpha = \overline{1, M}\ ,\quad M \geq 1\ ,\quad \beta = \overline{1, r}\ ,\quad r \geq 1\ ,$$

where φ is the function of state; $H_\alpha(\varphi)$ is the model of observations; the subscript α denotes the type of observations; M is the number of measuring, functionally different devices; $\xi_\alpha(\mathbf{x}, t)$ are the observation errors involving the errors of the device and the model itself. The superscript m is used for the parameters, which correspond to description of observations. The symbol $[\,]^m_\beta$ is used for the operation of information transfer from D_t or D_t^h to the point $(\mathbf{x}, t)_\beta$ of the set D_t^m. Usually it is the result of action of some operator of interpolation from D_t^h to D_t^m for the components of the functions, that is

$$[H_\alpha(\varphi)]_\beta = \hat{S}\ (H_\alpha(\varphi))\,\big|_{(\mathbf{x},\, t)_\beta}, \tag{2}$$

where $\hat{S}$ is the interpolation or projection operator.

Each component $\psi^m_{\alpha\beta}$ of the vector ψ^m is an individual value of the parameter at the point $(\mathbf{x}, t)_\beta$ measured by a method of the type α (from a given set of types). The structure of the vector ψ_m is defined as a block one, in which the type of observations determines the block number α, and the block itself is made up of the values measured by the method of this type at all points $(\mathbf{x}, t)_\beta$ of the area D_t, where the measurements are conducted.

Similarly to Eq. (1) we define the structure of vectors calculated using the model

$$[\psi]^m = \{[\psi]^m_{\alpha\beta} \equiv [H_\alpha(\varphi)]^m_\beta. \tag{3}$$

The operators of models of observations are selected to be bounded and differentiable with respect to the components of the vector function of state. Discrete analogs of these operators and operators $\hat{S}$ in Eq. (2) must have similar properties.

Models of processes and functionals of observations

Let us return to the problem of the relations between observations and basic models of the processes. The general methodology of modeling is based on two key elements.[3–5]

1. The mathematical model of the processes in the variational formulation is as follows:

$$I(\varphi,\, \varphi^*,\, \mathbf{Y})\ 0\ , \tag{4}$$

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

2. The set of functionals defined on the set of functions of state is

$$\Phi_k(\varphi) = \int\limits_{D_t} F_k(\varphi)\, \chi_k(\mathbf{x},\, t)\, \mathrm{d}D\, \mathrm{d}t,\quad k = \overline{1, K}\ ,\quad K \geq 1. \tag{5}$$

Here $I(\varphi, \varphi^*, \mathbf{Y})$ is the integral functional, which corresponds to the model in the differential formulation; φ is the function of state; $Q(D_t)$ is the space of functions satisfying the boundary conditions; φ^* are sufficiently smooth conjugate functions from the space $Q^*(D_t)$ conjugate to $Q(D_t)$; $\mathbf{Y}$ is the vector of input parameters of the model from the set of admissible values $R(D_t)$; $F_k(\varphi)$ are the preset scalar differentiable functions on the set of functions of state; $\chi_k(\mathbf{x}, t) \geq 0$ are the weighting functions generating Radon or Dirac measures in the domain D_t (Ref. 2). These measures are convenient for modeling because they provide for uniformly taking into account the fields of values of the functions in the functionals. These fields are distributed continuously and discretely in the domain D_t and can be taken into account either separately or in a combination.

The technique for construction of integral identities for models of the atmospheric and ocean physics, transfer and transformation of pollutants, as well as the methods of algorithmic arrangement of direct and inverse relations between functionals of type (5) and models in form (4) are sufficiently well developed.[3–6] Therefore, to arrange interaction between observations and models, it is sufficient to express the information about observations (1) and (2) in terms of the functionals of type (5) to include them into the modeling system.

The question arises here on what is it needed for. The point is that it is convenient to arrange the data of observations of different type arbitrarily spaced in the domain D_t in terms of functionals. For manipulation of functionals defined in D_t on the set of the functions of state, powerful mathematical apparatus of variational principles and conjugate problems is being applied. With this apparatus, every (even single) observation is related to the whole set of input parameters and external actions participating in the numerical models at any number of the internal degrees of freedom.

Consider equation (4) from the viewpoint of the theory of measurements. The weighting function $\chi_k(\mathbf{x}, t)$ in it can be interpreted as a function of deployment of the devices in the domain D_t. It determines the contribution of the function $F_k(\varphi)$ value at the point $(\mathbf{x}, t)$, which corresponds to a reading of the device set at this point, to the functional $\Phi_k(\varphi)$, that is, the resultant measured value of the parameter $F_k(\varphi(\mathbf{x}, t))$ in the domain D_t. The subscript k denotes the type of measurements. In particular, if χ_k is taken in the form of the Dirac delta function, then the value of the functional is equal to the value of the measured function at the point, which is the carrier of the weighting function.

Now, starting from definitions (1)–(3) and (5), we can form two types of functionals.

1. Functionals of “observationsB

$$\Phi_k(\varphi) = \int\limits_{D_t} H_\alpha(\varphi)\, \chi_{\alpha\beta}(\mathbf{x}, t)\, \mathrm{d}D\, \mathrm{d}t\ ,$$

$$k = \overline{1, K}\ , \quad K = Mr\ , \quad \{k\} \equiv \{\alpha, \beta\}\ , \qquad (6)$$

where $\chi_{\alpha\beta}(\mathbf{x}, t)$ are the preset weighting functions. If $\chi_{\alpha\beta}(\mathbf{x}, t)$ is equal to Dirac delta function with the carrier at the point $(\mathbf{x}, t)$, then the set of functionals (6) is the set of formulas for estimation of the components of vectors (1) and (3). Radon measures $\chi_{\alpha\beta}(\mathbf{x}, t)\,\mathrm{d}D\mathrm{d}t$ are of interest for practical application since they are taken as a sum of Dirac measures concentrated at a collection of points from the set D_t^m (Ref. 2).

2. Functionals of "quality."

The functionals of this type have a character of the discrepancy between the components of the vector of observations calculated using model (3) and under real conditions (1). They express the measure of errors $\xi_\alpha(\mathbf{x}, t)$ in Eq. (1) and are used in the problems of assimilation of the measured data with the use of models of the processes studied, diagnostics of the quality of models, and identification of their parameters and sources of external actions from the set of measured data.

The structure of the functionals of quality is defined by the following formulas:

$$\Phi_0^h(\varphi) = [([\psi]^m - \psi^m)^{\mathrm{T}}\, W_0([\psi]^m - \psi^m)]_{D_t^m}\ , \qquad (7)$$

$$\Phi_0(\varphi) = \sum_{\alpha=1}^{M} \int\limits_{D_t} \{W_\alpha([\hat{S}H_\alpha(\varphi)]^m - \psi_\alpha^m)\times$$

$$\times([\hat{S}H_\alpha(\varphi)]^m - \psi_\alpha^m)\}\, \chi_\alpha(\mathbf{x}, t)\, \mathrm{d}D\, \mathrm{d}t\ , \qquad (8)$$

where W_0 and W_α are the weighting matrices; χ_α are the weighting functions, $\chi_\alpha \mathrm{d}D\mathrm{d}t$ are Radon measures, which are chosen so that they allow for all components of the vector ψ^m; the subscript h is for the discrete analog; and T denotes the transposition. The scalar product in Eq. (7) is defined on the discrete set D_t^m. Given the measures are selected in such a way, the functionals in the form given by Eqs. (7) and (8) are equivalent in respect to the collection of observations.

The functional in form (8) has a wider spectrum of modifications than functional (7), because it allows selection of the weighting matrix and functions, measures, as well as of the operators $\hat{S}$.

When it is needed to combine the problems of data assimilation and that of identification of models with the problem of planning experiments in order to make the experiments more informative, the solution of such complex problems requires simultaneous use of both the functionals of "individual" observations (6) and functionals of quality (7) and (8).

Some relations of the theory of model and functional sensitivity

In order to finally solve the problem of inclusion of functionals into the technology of modeling, the algorithms of calculation of functions

$$\gamma_k^h(\varphi) \equiv \frac{\partial \Phi_k^h(\varphi)}{\partial \varphi}\ , \quad k = \overline{1, K}\ , \quad \varphi \in Q^h(D) \qquad (9)$$

are to be constructed. These functions are defined at the nodes of the grid domain D_t^h and take part, as sources, in the corresponding conjugate problems for the methods of inverse modeling and algorithms for studying sensitivity of models and functionals.

If some set of functionals is defined and the set of conjugate problems with sources (9) is constructed for it, then the main relations of sensitivity for these functionals are constructed by the algorithm[3,4]:

$$\delta\Phi_k^h(\varphi) = \frac{\partial}{\partial\zeta} I^h\,(\varphi,\,\varphi_k^*,\,\mathbf{Y} + \zeta\delta\mathbf{Y})\big|_{\zeta=0} \equiv$$

$$\equiv R^h(\varphi,\,\varphi_k^*,\,\delta\mathbf{Y})\,,\quad k = \overline{1,\,K}\,, \tag{10}$$

where I^h is the discrete analog of the functional of model (4); φ and φ^* are the solutions of the main and conjugate problems generated by the functionals I^h and $I^h + \Phi_k^h$, respectively; the symbol δ denotes variations of the corresponding parameter; ζ is the actual parameter. For example, for the model of atmospheric hydrothermodynamics combined with the model of transfer and transformation of pollutants accepted as a basis for solution of climatic and ecological problems of monitoring and prediction,[5] equations (10) have the form:

$$\delta\Phi_k(\varphi) = \left(\frac{\partial I(\varphi,\,\varphi_k^*,\,\mathbf{Y})}{\partial\mathbf{Y}}\,,\,\delta\mathbf{Y}\right) \equiv R(\varphi,\,\varphi_k^*,\,\delta\mathbf{Y}) =$$

$$= \int\limits_{D_t} \{c_3\delta Q_T T_k^* + c_4\delta Q_q q_k^* +$$

$$+ \sum_{\alpha=1}^{n} c_{\alpha+4}[\delta Q_{c\alpha} - \delta(B(\mathbf{C}))]_\alpha\}\,\mathrm{d}D\,\mathrm{d}t +$$

$$+ \int\limits_{D} \sum_{i=1}^{4+n} c_i\delta\psi_i\varphi_i^*\big|_{t=0} m\mathrm{d}D + R_1(\varphi,\,\varphi_k^*,\,\delta\mathbf{Y}) +$$

$$+ R_2(\varphi,\,\varphi_k^*,\,\delta\mathbf{Y}) + R_3(\varphi,\,\varphi_k^*,\,\delta\mathbf{Y})\,, \tag{11}$$

where R_1, R_2, and R_3 have the form:

$$R_1(\varphi,\,\varphi_k^*,\,\delta\mathbf{Y}) \equiv \int\limits_{\Omega_t} \Bigg\{\delta U_n \sum_{i=1}^{4+n} c_i\psi_i\varphi_{ik}^* \frac{m^2}{\pi} +$$

$$+ \sum_{i=1}^{4+n} c_i U_n \delta\psi_i\varphi_{ik}^* \frac{m^2}{\pi} - \frac{\delta\pi}{\pi^2} \sum_{i=1}^{4+n} m^2 c_i U_n \psi_i \varphi_{ik}^*\Bigg\}\,\mathrm{d}\Omega\,\mathrm{d}t\,, \tag{12}$$

$$R_2(\varphi,\,\varphi_k^*,\,\delta\mathbf{Y}) \equiv$$

$$\equiv \sum_{i=1}^{4+n} c_i \Bigg\{\int\limits_{D_t}\Big[\delta\mu_i \mathrm{grad}_s\psi_i \mathrm{grad}_s\varphi_{ik}^* + \frac{\delta v_i}{m}\frac{\partial\psi_i}{\partial\sigma}\frac{\partial\varphi_{ik}^*}{\partial\sigma}\Big] m^2\mathrm{d}D\mathrm{d}t +$$

$$+ \int\limits_{\Omega_t} \delta r_i \varphi_{ik}^* m\mathrm{d}\Omega\mathrm{d}t + \int\limits_{S_t} \delta\tau_i\,\varphi_{ik}^* m\mathrm{d}S\,\mathrm{d}t\Bigg\}\,, \tag{13}$$

$$R_3(\varphi,\,\varphi_k^*,\,\delta\mathbf{Y}) \equiv$$

$$\equiv \int\limits_{\Omega_t} \{G_k^*\delta U_n + U_{nk}^*\delta G + (U_{nk}^* - U_n T_k^*)\delta\pi -$$

$$- \pi T_k^*\delta U_n\}\, m\,\mathrm{d}\Omega\,\mathrm{d}t - \int\limits_{S} T_k^*\delta(G_s\pi) + \pi_k^*\delta\pi\big|_{t=0}\,\mathrm{d}S\,. \tag{14}$$

Here we use the designations from Refs. 5 and 6:

$$\varphi = \{\varphi_i,\,(i = \overline{1,\,4+n}\,\} \equiv \{u,\,v,\,T,\,q,\,C_\alpha\,(\alpha = \overline{1,\,n}\,)\}$$

are some functions of state of the basic model; $\psi = (\pi/m)\varphi$; the asterisk denotes the corresponding components of the conjugate functions; U_n is the component of a velocity vector $\mathbf{U} = (\pi/m)\times\,(u,\,v,\,\dot\sigma)$ normal to the boundary Ω_t of the domain D_t; S_t is the projection of the domain D_t onto the Earth's surface; u, v, and $\dot\sigma$ are the components of the velocity vector along the directions of the coordinate axes x, y, and σ, respectively; T is the temperature; q is the specific humidity; C_α is the pollutant concentration; n is the number of different pollutants; G is the geopotential; π is the function of pressure; m is the scaling factor of the coordinate system; dD, dΩ, and dS are the elementary volumes and areas; c_i ($i = \overline{1,\,4+n}$) are the weight coefficients to fit the physical dimensionality of terms in the integral identity of model (4); μ_i and ν_i are the coefficients of horizontal and vertical exchange for the pollutant i; r_i and τ_i are the turbulent flows at the boundaries Ω_t and S_t. The symbol δ in the right-hand sides of Eqs. (11)–(14) denotes variations of the input (relative to the model) parameters: components of the vector of state φ, ψ, $(\delta\psi_i = \pi\delta\varphi_i + \varphi_i\delta\pi)/m$, $\delta\varphi_i = (m\delta\psi_i - \varphi_i\delta\pi)/\pi)$, the vector of parameters $\mathbf{Y}$, the sources of heat Q_T, humidity Q_q, and pollutants Q_C. The term $\delta(B(\mathbf{C}))$ means the variation of the operator of pollutant transformation because of variations of rate constants of reactions included into the operator. The terms containing variations of heat influx δQ_T depend on variations of concentrations of optically active gases. For their calculation, the complex basic model of hydrothermodynamics with the radiative block is considered in combination with the model of pollutant transport. In this case, a new type of conjugate equation arises as a part of the model of pollutant transfer. The new point is the appearance of terms allowing for information about tendencies in the influence of inhomogeneities in concentrations of optically active gases on the radiative processes. Besides, a new element arises in the basic models. It is the system of equations conjugate with respect to the radiative block. The formulas for calculation of the corresponding additional, to formulas (11)–(14), expressions are given in Ref. 7.

Equations (11)–(14) show (at the informative level) the character of relations of functionals to the parameters and external sources. The coefficients entering into Eqs. (11)–(14) as the factors at variations of the input data have the meaning of the functions of sensitivity of the functional $\Phi_k(\varphi)$ to the corresponding variations.

Thus, we have completely developed the "inner" algorithmic cycle for combining the models and data of observations. With the use of the functions of sensitivity, the methods of direct and inverse modeling are realized within the framework of the general methodology of modeling described in Refs. 3 and 4.

Conclusion

This paper presents the conceptual and algorithmic problems of combining the experimental and theoretical knowledge expressed in the data of observations and in mathematical models for investigations into the atmospheric processes jointly with the processes of transfer and transformation of pollutants. An example of such combining is given by the relations of the theory of sensitivity for the functionals containing measured data. These relations are the basic point for the development of methods of inverse modeling. These methods provide for relating the information to a model. They involve the conjugate problems for the functionals of the class under consideration. These problems can have independent importance when studying scales and the character of interaction in a climatic system functioning under the influence of natural and anthropogenic factors.

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