A variational approach to environmental and climatic problems of urban agglomerations

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Abstract. We discuss some aspects of the development of a variational approach to study the dynamics of climatic and ecological systems under intensive actions of natural and anthropogenic origin. The variational principle essentially represents a versatile tool to create a consistent modeling technology based on models of processes coupled with available observational data. The basic entities included in the formulation of the variational principle are models of processes; data and models of observations; target criteria for forecasting; a priori information about all the required elements of the system. We develop a set of mathematical models combined within the framework of the variational principle. They describe the dynamics of the atmosphere and water bodies in conjunction with a thermally and dynamically heterogeneous surface of the Earth; the hydrological cycle, moisture in the atmosphere and the soil; radiation transfer in the system of the atmosphere and the underlying surface; and transport and transformation of various substances in gaseous and aerosol states in the atmosphere. As an example, we demonstrate the results of calculations performed with a set of numerical models adapted to the conditions of a Novosibirsk city agglomeration. The results of scenario calculations on the formation of mesoclimates and quality of the atmosphere for the typical conditions of Siberian cities are presented.

1. Introduction

Throughout the history of mankind, compact residences have been sought in limited areas selected under various criteria. People interact with natural environment, use its resources and, quite frequently, exhaust them. Currently, the results of this interaction are clearly visible, especially in urban agglomerations and industrial regions. Therefore, the studies of problems arising in the interaction with the environment occupy an increasingly prominent place in the research on environmental problems. Now such studies are difficult without the use of mathematical modeling.

Here we discuss some applications of a variational approach to study problems which are critical in the theory of climate and the environment [1-5]. The results of their solutions provide a direct contribution to the sphere of practical applications. These are the assessment of the impact on human health, environmental safety, and the organization of environmental policies. To solve them, mathematical models and technical means for monitoring the parameters of the processes are being developed in many scientific centers of the world [6,7].

Methods for solving environmental problems based on coupled models of dynamics and atmospheric chemistry have been developed at ICM&MG SB RAS since 1980 [2,5]. Descriptions of the variational modeling technologies and some new versions of the models of this class are given in [8,9]. We proceed from the premise that the mathematical models and monitoring systems describe the evolution of the same processes and objects, but by different means. Their union is based on variational data assimilation methods [4, 9-10]. Essentially, the variational principles are a universal tool for creating a consistent modeling technology based on the use of process models coupled with available observational data. Contemporary reviews of works on this subject can be found in [7,11,12] and in the bibliography available there.

2. Statement of the problems

To conduct research and to solve practical problems we use a variational approach that combines all the elements of the technology of mathematical modelling. The core objects included in the formulation of the variational principle are: process models; observed data and models of observations; a priori information about all the required elements of the simulation system; target criteria for prediction and design; functional limitations on the quality of the environment and sanitary conditions and environmental standards for the quality of life and health of the population of urban agglomerations.

Consistency is an important factor for the processes of different scales and different nature in conditions of uncertainty, both in the models and in the observational data. To solve this class of problems, we use the following set of mathematical models: hydrodynamics of geophysical fluids (for air and water bodies) in conjunction with a thermally and dynamically inhomogeneous surface of the Earth; the hydrological cycle of moisture transformation in the atmosphere; heat and moisture transport in the soil; radiative transfer in the system of the atmosphere and the underlying surface; transport and transformation of various substances in gaseous and aerosol states in the atmosphere.

Chemically, optically, and thermodynamically active substances, biologically active aerosols and radionuclides are of special interest for practical applications. Secondary products of transformations of primary emissions from the sources affect human health, the quality of air and water, as well as the state of ecosystems. They require special attention.

It should be noted that the whole set of multifunctional factors and different substances manifests itself in an integrated form in the living space of urban agglomerations and may have synergetic effects of their interactions. Therefore, the main issues are to identify the internal mechanisms of the formation and evolution of processes as well as to evaluate possible changes in the quality of the environment for a long period. These changes may occur not only as a result of work of the existing enterprises, but also from new objects of further economic developments of the territories. Moreover, we are interested in possible changes not only in the metropolitan area, but also beyond it, in the areas of risk / vulnerability for the region being studied.

Given these preconditions for the organization of simulation scenarios, we evaluate the extent of interactions in the global climatic system and in the region where the objects being studied are located. For these purposes, we use methods of scale decomposition of the investigated phenomena and evaluation of the characteristic times and intensities of the sources of impact in the region. They allow us to create a set of scripts to reproduce typical meso-regional climates on the background of the global circulation mechanisms [13].

The mathematical models for studying the atmospheric processes mentioned above are represented by systems of equations of hydrodynamics. They are unsteady in time and three-dimensional in space. We study the behaviour of various substances in gas and aerosol states with the help of equations of the convection-diffusion-reaction type. To combine them into a generalized system, we design a main functional of integral identity which acts as restrictions on a class of functions in the generalized formulation of the variational principle. For definiteness, we choose a form of the functional based on the structure of a balance equation for the total energy of the system. Observational data are also included in the system within the framework of a variational principle. This is done by means of special functionals expressing a measure of deviations between the observations and their images, which are calculated by the models of observations with the sought functions of state.

A general structure of the modeling technology is presented in [8-10,14]. The numerical implementation of the variational principles is carried out with functional decomposition and splitting methods for the operators of the process models [1,4,15]. For the construction of numerical schemes we have developed discrete-analytical methods based on a concept of adjoint integration multipliers (factors) [16]. Such methods are convenient for the study of multi-scale and multi-parameter processes with high spatial-temporal resolution, without increasing the dimensions of the grid domains.

3. Variational organization of the modelling system

Uncertainties of various kinds are always present in the process models and the observational data. Under an uncertainty we mean the errors of observations, the lack of modern knowledge about the natural processes and their representation in the models. To account for them we introduce additional unknown functions into the model. They represent a quantitative measure of uncertainty in the relevant model equations, in the parameterizations of physical processes, and in the input data and sources. The fundamental importance of these functions is that they provide a quantitative assessment of the degree of conformity of the results of calculations by the models to the results of monitoring the behavior of the real system. In this formulation, the models are not exact. Therefore, we build the variational principle in a weak-constraint formulation. A variety of assessments of the effects of uncertainties for research and practical purposes are being developed in the world (see reviews in [10-12]).

We develop a computationally efficient version of the variational approach with assimilation of observed data. The weak-constraint formulation of the variational principle is equivalent to well-known approaches such as variational methods with weighted least squares of Gauss, including Tikhonov regularization; variational principles of Euler-Lagrange with the technique of Lagrange multipliers, and methods like Kalman filtering.

An advantage of our approach is the use of more efficient algorithms, especially in sequential data assimilation technique with splitting and decomposition methods [9,10]. This allows us to build a forecasting system with non-iterative (direct) data assimilation algorithms allowing a parallel organization of the calculations. The computational efficiency of direct algorithms increases, as compared to the other approaches for solving the problems of data assimilation, with increasing volume of observations in space and time.

The purpose of the study and the sequence of operations when implementing the variational approach define the set of its basic elements:

- the systems of equations in numerical models:
  - ✓ main (forward mode),
  - ✓ adjoint (backward in time),
  - ✓ for calculation of uncertainty functions;
- the set of algorithms:
  - ✓ formation of operators of model sensitivity to variations of all the parameters, sources of influence, and other objects,
  - ✓ calculation of sensitivity functions of the objective functional using the solutions of the main and adjoint problems, and uncertainty functions,
  - ✓ data assimilation and regularization for solving inverse problems,
  - ✓ feedback for the solution of inverse problems for identification of sources of influence and model parameters with respect to specified target criteria and constraints,
  - ✓ estimation of the functions and areas of risk/vulnerability of the object-receptors in relation to existing and potential sources of heat and pollution.

The problem of identifying the active energy centers of action on various spatial-temporal scales is of great interest in the study of critical issues of climatic and ecological systems of the Earth and its specific regions. First of all, on the basis of mathematical models we need to clarify the place of an object in a climatic and ecological system and evaluate its role as a source and receptor of influence in this system. The above-mentioned methods allow us to calculate functions of risk and vulnerability of these objects against the effects of potentially dangerous sources in the region. Therefore, for solving problems of this class we develop a technology of mathematical modeling which involves models of different physical content and spatial-temporal scales. Methods of constructing numerical schemes and algorithms for implementing the mathematical models based on a variational concept of adjoint integrating factors provide sufficient accuracy of approximations for a wide range of spatial-temporal resolutions of the models [16].

4. Adaptive targeted monitoring strategy

We develop a scenario approach based on variational methods for the formation of targeted monitoring strategies and planning of observational experiments. In relation to the problem of forecasting the dynamics of the processes and changes in the quality of the atmosphere, this is a versatile research tool for solving a sequence of inverse problems.

Methods of implementing such an information technology are proposed in [13]. We combine methods of scale decomposition of the processes being studied and methods of model sensitivity with assessment of uncertainty in the modeling technique. To this end, we conduct a joint analysis of multidimensional fields of the state functions, adjoint functions, uncertainty functions and a set of sensitivity functions of objective (cost) prognostic functionals.

We use methods of orthogonal decomposition of multidimensional spaces of functions based on singular value decomposition methods to identify the main factors and centers of action with an estimate of characteristic scales of their intensity. The result is a system of informative basis subspaces that are ranked according to some criteria of informativeness of the singular values.

In this way it is possible to separate the subspaces of climatically significant scale from the subspaces of weather noise [13]. Their knowledge is useful when solving practical problems of ecological safety and environmental design for a long period. Such bases are also used in the operational methods of a few-parameter reconstruction of state functions with assimilation of observational data in real time. In particular, if we design new facilities related to emissions of heat, moisture, and pollutants, as well as to changes in the characteristics of the underlying surface, this increases the information content of climate scenarios to obtain estimates of environmental perspectives in the region for a long time.

5. A scenario for the Novosibirsk city agglomeration

The seventh in Russia, the city of Novosibirsk (1.7—2.0 million people) is the most important inter-regional center of social and economic development and an attractor for the macro-region of Western Siberia. The cities of Berdsk, Iskitim, Ob, and major scientific centers-satellites of Novosibirsk, Koltsovo, and Krasnoobsk are the main parts of the Novosibirsk agglomeration. Akademgorodok is one of the districts of the city of Novosibirsk.

This industrial area is characterized by a high level of anthropogenic load. The main climatic factor of meso-regional scale is formed as a result of the hydrodynamic and environmental interactions of the objects of Novosibirsk agglomeration with two main water bodies, the Ob river and the reservoir of the Novosibirsk hydroelectric power station. This climatic factor manifests itself continuously in the form of daily and seasonal variations on the background of global processes.

As an example, we present the simulation results of a typical scenario of the formation of mesoclimates in the region under the influence of a background flow, as well as the fields of pollutant concentrations constructed by these mesoclimates.

In the calculations, we use a set of meso-regional models describing the hydrodynamics, transport, and transformation of pollutants adapted to the conditions of the Novosibirsk agglomeration. The system of equations of the models and methods of their realization are described in [8,10,16]. The dynamic model takes into account the processes of hydrological cycle. A parameterization of the processes in the atmospheric surface layer and the main surface heterogeneity are considered as well.

Some land use categories in the region are taken into account: city, river, reservoir, different kinds of forests and farmland.

In the scenario, the circulation of the atmosphere is formed under the influence of a south-western background flow with a wind speed of about 8 m/s given at a height of 3000 m above the ground. Diurnal solar radiation for the summer season is also included. The urban agglomeration is considered as a set of distributed sources of anthropogenic pollution and as a generator of "heat islands" in the atmosphere that interact with the environment. The sources of pollutants and artificial heat fluxes are defined in a parameterized form in view of the intensity of human activity and traffic flows within the metropolitan area.

The results of some scenario calculations on the formation of mesoclimates and air quality for the Novosibirsk agglomeration at two time points are shown in figures 1 and 2. Two-dimensional cross-sections of the fields of concentrations of pollutants and velocity vector at 07:00 a.m. local time are given in figure1. On the left plot (a), a horizontal section at the level of the surface layer is shown. The right plot (b) demonstrates a vertical cross-section through the central part of the city of Novosibirsk along the coordinate line $y = 65\text{km}$. The same cross-sections at 06.00 p.m. local time are shown in figure 2.

Analysis of the results of the scenario calculations has shown that specific local circulation systems are formed in the agglomeration due to the contrasts between the warm and cold areas. The characteristic scales of influence domains of urban heat islands are about 20 km in the horizontal directions and from 500 m to 2 km in the vertical direction.

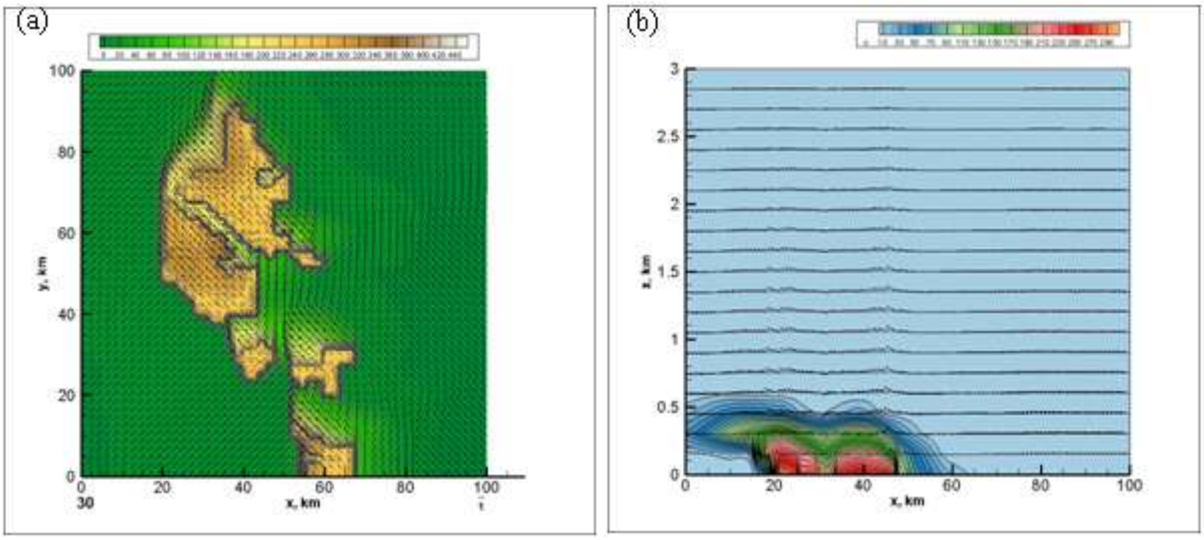

Figure 1. Concentration of pollutant (relative units) and velocity vector (m/s) at 7:00 a.m. local time. A 2D horizontal section at the level of the surface layer (a), and a vertical section through the central part of Novosibirsk city (b).

The cold river divides the greatest heat island into two parts. In the daily and seasonal variations, areas of high levels of pollutant concentrations are generated above the urban territories. In the vicinities of the bounds between the city and the surroundings the effects of internal boundary layers manifest themselves in the structure of fields of the state functions. Accordingly, we observe some wave behavior in the space-time dynamics of the fields of wind, temperature, and concentrations of pollutants.

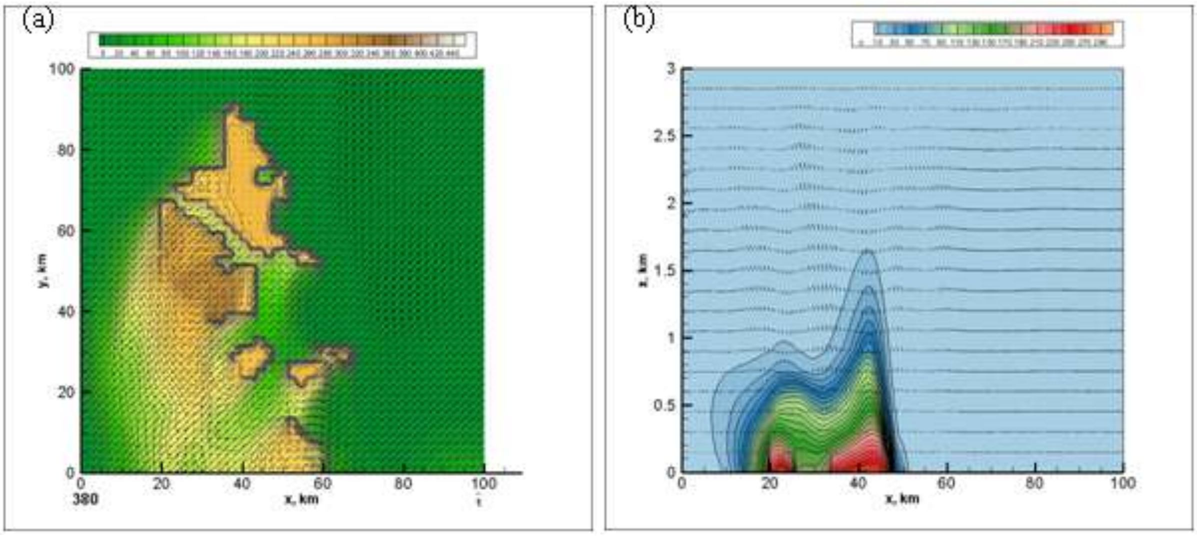

Figure 2. The same as in figure1 but for 06.00 p.m. local time.

6. Conclusions

Modelling systems of the processes on urban and meso-regional scales are necessary tools for the evaluation of actual status and quality control in normal and especially in emergency situations in urban areas. The scenario approach allows us to explore a variety of climatic and environmental situations in specific conditions of the region under study. With this type of a system, we can solve a variety of inverse problems, including the calculation of risk functions, assessment of the impact of emergency situations with identification of the exposure sources. These systems are of particular importance for a long-term environmental design of the construction and operation modes of objects that represent a potential hazard to the people and the environment.

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References

[1] Marchuk G I 1974 *Numerical Solution of Atmospheric and Oceanic Problems* (Leningrad: Gidgometeoizdat) p 303
[2] Marchuk G I 1982 *Mathematical Models in Environmental Problems* (Moscow: Nauka) p 319
[3] Marchuk G I 1992 *Adjoint Equations and Analysis of Complex Systems* (Moscow: Nauka) p 334
[4] Penenko V V 1981 *Methods for Numerical Modeling of Atmospheric Processes* (Leningrad: Gidrometeoizdat) p 352
[5] Penenko V V, Aloyan A E 1985 *Models and Methods for Envronmental Protection Problems* (Novosibirsk:Nauka) p.256
[6] Baklanov A, Machura A, and Sokhi R 2011 *Integrated Systems of Meso-meteorological and Chemical Transport Models*. (Heidelberg Dordrecht: Springer) p 242
[7] *Seamless Prediction of the Earth System: from Minutes to Months* 2015 WMO-No.1156
[8] Penenko V V, Tsvetova E A and Penenko A V 2015 *Izvestiya, Atmospheric and Oceanic Physics* **51** pp 311–19
[9] Penenko V V, Tsvetova E A and Penenko A V 2015 *Russian Meteorology and Hydrology* **40**

pp 365-73
[10] Penenko V V 2009 *Numer. Anal. Appl.* **2** pp 341–51
[11] Navon I M 2009 *Data Assimilation for Atmospheric, Oceanic and Hydrologic Appl.* **1** pp 21-65
[12] Bocquet M et al. 2015, *Atmos. Chem. Phys.*, **15** pp 5325-58
[13] Penenko V and Tsvetova E 2008 *Ecol. Modell.* **217**, 279–291
[14] Penenko V, Baklanov A, Tsvetova E. and Mahura A. 2012 *Pure and Applied Geoph.* **169** pp 447-65
[15] Samarskii A A, Vabishevich P N 2001 *Additive Schemes for Problems of Mathematical Physics* (Moscow: Nauka) p 319
[16] Penenko V V, Tsvetova E A and Penenko A V 2014 *Comp. & Math. with Appl.* **67**, pp 2240–56.