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Enviro-RISKS:

Man-induced Environmental Risks: Monitoring, Management and Remediation of Man-made Changes in Siberia

Alexander Baklanov and Evgeny Gordov, Editors

Volume 2:

Atmospheric Pollution and Risk

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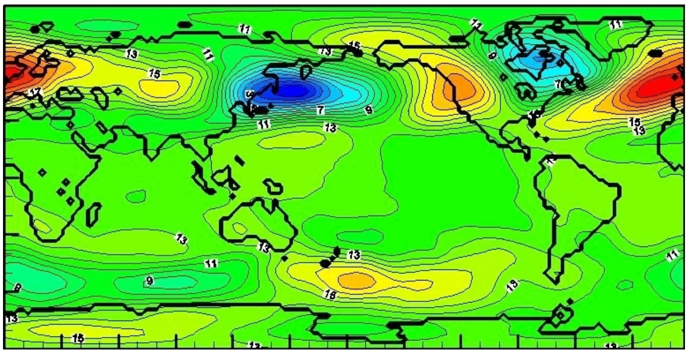

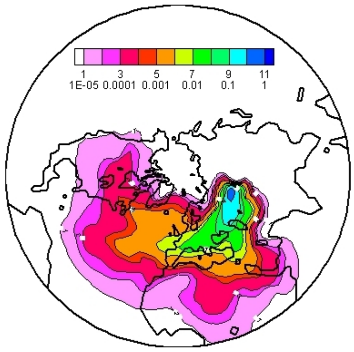

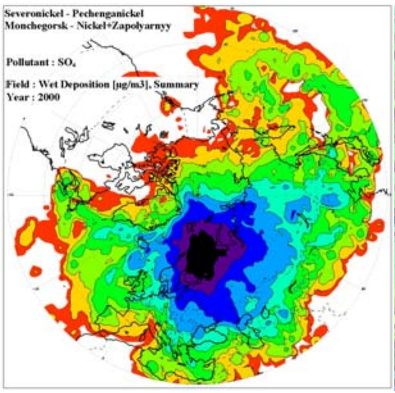

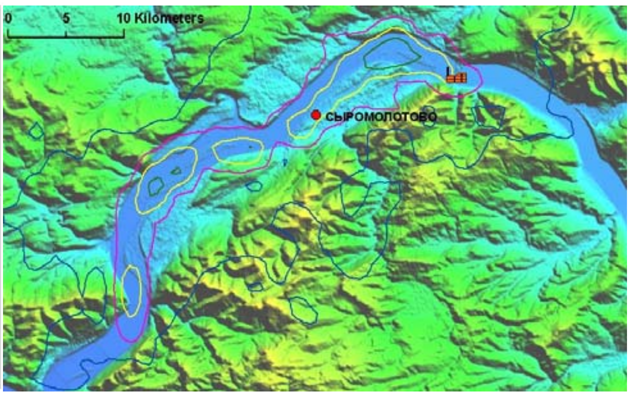

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Enviro-RISKS Report Content:

Executive Summary

Enviro-RISKS Project and its Major Outputs *(in a separate Volume1:* www.dmi.dk/dmi/sr08-05-1.pdf*)*

Thematic Focus 1: Atmospheric Pollution and Risk *(in this Volume 2)*

Thematic Focus 2: Climate/Global Change and Risks *(in a separate Volume 3:* www.dmi.dk/dmi/sr08-05-3.pdf*)*

Thematic Focus 3: Terrestrial Ecosystems and Hydrology and Risks *(in a separate Volume 4:* www.dmi.dk/dmi/sr08-05-4.pdf*)*

Thematic Focus 4: Information Systems, Integration and Synthesis *(in a separate Volume 5:* www.dmi.dk/dmi/sr08-05-5.pdf*)*

EXECUTIVE SUMMARY

Siberia environment has been subjected to serious man-made transformations during last 50 years. Current regional level environmental risks are: direct damages to environment caused by accidents in process of petroleum/gas production and transporting including their influence on water, soil, vegetation and animals; caused by deforestation (legal and illegal cutting and forest fires) variations in Siberian rivers runoffs and wetland regimes; direct and indirect influence of forest fires, flambeau lights and losses of gas and petroleum during their transportation on regional atmosphere composition; deposition of hazardous species leading to risks to soil, water and consequently to risks in the food chain.

In this Final Report, published in five separate Volumes, the major Enviro-RISKS project (http://project.risks.scert.ru/) outcomes are summarized. They include the state of the art of environmental RTD activity in Siberia, suggested methodology and recommendations on future environmental research in Siberia. These outcomes are based on results obtained by the four Thematic Expert Groups in process of preparation of Thematic Focuses Reports.
Three Thematic Focuses/Groups consider major risks inherent to Siberia environment. These groups (with their leaders) are the following:

1. **Atmospheric Pollution and Risks** (Alexander Baklanov (DMI) and Vladimir Penenko (ICMMG)),
2. **Climate/Global Change and Risks** (Martin Heimann (MPI for Biogeochemistry) and Vasily Lykosov (INM)), and
3. **Terrestrial Ecosystems and Hydrology and Risks** (Michael Kabanov (IMCES) and Anatoly Shvidenko (IIASA)).

The forth Focus has a generic nature and is devoted to:

4. **Information Systems for Environmental Sciences, Integration and Synthesis** (Evgeny Gordov (SCERT) and Edige Zakarin (KGC)).

The groups analyzed relevant RTD projects (lists of those are mentioned in the Introduction and attached to respective Focus Groups Reports) and summarized the state of the art, existing methodology and applications in the considered area. Additional contributions of all Project Partners also have been used in this Report.
On this basis also practical recommendation to international research community and regional environmental decision makers were formulated (see in Volume 1). These recommendations are translated into Russian and disseminated to targeted community via direct mailing and the Project web site.

Content of Volume 2: Atmospheric Pollution and Risk:

Abstract

The major results of the first **Thematic Focus** and relevant **Working Group** of **Atmospheric Pollution and Risks** inherent to Siberia environment are described in this Volume 1 of the Final Scientific Report of the EC FP6 Coordination Action of Enviro-RISKS: Man-induced Environmental Risks: Monitoring, Management and Remediation of Man-made Changes in Siberia. The main focus was done on the current state and strategic activities in risk assessment and environmental modelling in Siberia, a modern concept of environmental modelling, including online integrated approach, variational principles, forward and inverse modeling and sensitivity studies. Some practical recommendations for organization and implementation of environmental models, as well as a few examples of current studies of applied environmental problems in Siberia, based on the Enviro-RISKS CA and involved projects, are also presented in this Report.

Introduction

To sketch a scope of environmental problems of Siberian cities, it is necessary to underline the following. Essential dependence of atmospheric quality from climatic conditions is typical for Siberian cities. A stable atmospheric stratification and temperature inversions are predominant weather patterns for more than half a year. This contributes to accumulation of pollutants of different nature in the low layers of the atmosphere namely where ecosystems function and people live.
In addition to the severe climatic conditions, man-made impacts on environment in industrial cities strengthen more and more. The impacts manifest themselves in pollution of environment, change of the Earth surface, of hydrological and hydrodynamic regimes of the atmosphere, etc.
In the cities, original meso-climates form that promote pollution accumulation. Urban cenosis develop there in the extreme and evolutionary non-providing conditions. Therefore they are peculiar and weakly studied ecosystem types. Here the natural and industrial (energy, transport) complexes are closely connected. There are severe contradictions between the growing chemistry components in all branches of industry and the low level of general chemistry competence even at a level of decision-making of high responsibility. For example, the unfinished technologies without of final stages of the wastes use are often realized till now. That is why a potential risk of man-made catastrophes is high. The latter may in their turn provoke ecological disasters by atmospheric emission of heat, humidity, and toxic pollutants.
It should be noted that cities are not isolated systems. They may as distribute pollution over surroundings as get it from the outside. Thus the problem of mutual risk assessment for the cities should not be underestimated in the specific Siberian conditions, too. The influence of the transboundary transport between Russia, China, Kazakhstan, and Mongolia should not be ignored as well. All these problems are connected with ecological safety and life quality.
Now the close connection between environment quality and man's health, working capacity and life time is beyond any doubt. A general worsening of ecological situation in Siberian cities causes its input to the accumulation of the toxic products in the organs and tissues of men. This reflects in the functioning of the organism as a whole and leads to the metabolic imbalance.
There are both the own ecological and environmental problems in Siberian and Kazakhstan cities and the typical problems for many of them. For instance, Novosibirsk, Krasnoyarsk, Irkutsk, Ulan-Ude, Ust'-Kamenogorsk are in the influence zones of the meso-climates provided by the interplay of the city heat island and the water objects. This increases vulnerability of the atmospheric quality to the pollution. These aspects demand additional studies while planning the economical activity.
One more important fact is that the cities of West Siberia are situated in the influence regions of the vast wetland (bog) territories of the gas-oil provinces where methane is naturally emitted into the atmosphere. We know methane as a greenhouse gas. Hence, the problems of climate change are directly concerned with Siberia. Moreover, the emission resulted from mining and processing hydrocarbons is added to increase the concentrations. It is known that series of toxic secondary products such as formaldehyde, formic acid, etc. is generated when methane transforms. It is not quite clear till now to what extent does this neighborhood be dangerous for Siberian people.

1. Current State and Strategic Activities

1.1. Peculiarity of environmental protection problems

The statements of environmental protection problems are varied because this field of science is based on the knowledge and methods of a number of disciplines like physics, chemistry, ecology, economy, mathematics and others. The developing mathematical tools should be intended for integration of heterogeneous knowledge in an agreed system.

Traditional approaches to the solution of environmental protection problems are usually based on the methods of forward (direct) modelling. Their essence is in the construction of the models and scenario calculations under different choice of input data and external impact. In spite of the wide spread of such approach, it cannot provide the whole range of problems at contemporary level. First of all, this concerns with the problems of design and control.

The specific feature of this class of problems is the fact that it is necessary to consider a wide range of interconnecting processes for a long time intervals in the regions of different scales with uncertainties in external and internal sources of perturbations. Not each source of pollution is known. Besides, there is an evidence on uncertainties in weather and in the climate system behavior. We should not dismiss the possibilities of back relations when the changes in the climatic system are the result of man-made or natural pollution. Thus, accounting direct relations and feedback effects is dictated by the peculiarities of the class of problems.

1.2. Risk assessment problem

Concepts of risk and vulnerability of territories with respect to natural and man-made impacts are of fundamental significance in ecological and environmental studies. Risk investigation is concurrent part of the problems of ecological prognosis and design which are on the edge of biosphere and climate science.
We should not exclude the unintended impacts, the natural and industrial, connected with intensive emissions of heat, humidity and pollutants. The consequences of war conflicts and terrorist acts are ranged as the high risk situations, too.
World experience shows that the danger of large scale industrial catastrophes increases, as a rule, when the technical complexity and energy capacity grow. More and more often these catastrophes lead to severe ecological consequences. A critical situation may be evolved from the whole set of problems in Siberian regions of Russia where pollution accumulates in the low levels of the atmosphere owing to the climatic conditions and where the preferential orientation of industry to mine raw material, has been developing for a long time.
Recent trends in environment protection are towards increased use of numerical modelling for risk assessment. With the help of models, one can reveal the potentially hazardous situations and objects, quantitatively estimate the heaviness degree of the consequences of catastrophic events.
The goal of the research for modern period we see in the retrieval of constructive solutions for management of the environment quality including the risk control and design of the environmental protection and social actions on prevention and mitigation of negative consequences being due to the fact of deliberate and unintended influences.

1.3. Tendencies in environmental modelling in Siberia

Environmental problems are under study of Siberian scientists. As our thematic group in the project concerns with atmospheric pollution and risk, we concentrate on numerical modelling in these fields giving the proper attention to the close connection between climatic and environmental problems.
There are some leading groups of environmental modelers in Novosibirsk, Tomsk, Irkutsk, Krasnoyarsk, Tumen, Barnaul, Kemerovo, Yakutsk, Ulan-Ude, Chita, Omsk, and Khanti-Mansiisk. These groups belong mainly to the institutes of the Siberian Department of the Russian Academy of Sciences.
There are three tendencies in the usage of modelling tools in these groups:

- using simplified regulatory models (Gaussian type, one/two dimensions, a few parameters, etc.), (about 50-60 %)
- adopting well-known internet-available models, like MM5, WRF, HYSPLIT, etc. (20-30 %, increasing)
- developing original comprehensive models of different complexity from local to global scales (10-15%, decreasing).

The following description is mainly focused on the approaches developed by the participants of the present project.

A system for modelling dynamics and pollution in Tomsk region is developed by Tomsk State University, IAO and IMCES SB RAS. The models MM5, WRF and an original version of non-hydrostatic meso-scale hydrodynamic model as well as the model of transport and transformation of substances are used. Photochemical reactions are also considered in the air quality models for urban and suburban areas. Special attention is given to the parallel realization of the models and high performance numerical schemes (Starchenko, 2003, Starchenko et al., 2005).

In KazGeoCosmos, a geo-informative system for simulation of a city and industrial region pollution is elaborated. A 2D model of pollutant transport is included into it. The model is adapted to the Alma-Ata city conditions. A special version of the model is developed for assessment of the atmospheric quality in Kazakhstan's sector of Caspian region. The main part of emission is the products of burning at processing hydrocarbons. The emergency cases are considered too (Zakarin, Zakarin and Mirkarimova).
In ICMMG, a set of atmospheric models of environmental orientation (CARMEN) has been developed. Under a concept of ecological modelling accepted there, the model set is hierarchically constructed in such a way that the basic models of some vertical and horizontal scales participate in it. The models are of local, meso, hemispheric and global scales. The adjustment of the models is fulfilled by variational principles. A methodology has been developed to build the combined methods of forward and inverse modelling for the problems of the higher system level connected with the problems of ecological safety and environment control. The methodology includes the basic elements for calculation of sensitivity functions to the variations of input data, parameters, and sources. Mathematical aspects of methodology, statements of the problems, and modelling technology are described in (Penenko, 1981, Penenko and Tsvetova). The essence of the concept is shortly given below.

2. A Concept of Environmental Modelling

Environmental modelling has been developing in ICMMG of SD RAS (former Computing Center of the Siberian Division of the USSR Academy of Sciences) since the seventieth years of the last century. The very important merit of G.I.Marchuk, the first director of the institute and the leader of the Department of atmospheric and ocean studies, was introduction of adjoint equations into the theory and practice of the mathematical modelling of the ocean, atmospheric and environmental dynamics. In his monographs (Marchuk, 1974, 1982, 1994) one can find the basic ideas of fundamental approaches and a great number of numerical schemes and algorithms.

A concept of environment modelling started in works (Penenko, 1975; 1981) uses and enhances the adjoint methodology. It is based on variational principles and adjoint sensitivity theory. This allows one to obtain the optimal numerical schemes and the universal algorithm of the forward and inverse modelling. Since then the methodology has been developing till nowadays (see Penenko and Aloyan, 1985, and the other works of Penenko and Penenko with co-authors given in the list of references). This methodology was further developed and applied by a number of scientists, which were grows in this Novosibirsk scientific school (see e.g., Baklanov, 1988; 1990; 2000).

Following the concept, the constructions in the form of functionals describing the generalized characteristics of the processes, data, and models are considered together with the basic model components. Ecological restrictions on the environment quality, the results of measurements of different kinds, control and design criteria, model quality criteria, etc. are presented by the functionals. The restriction functionals are introduced for solving the problems of optimisation of environment protection activity, management of environment quality, and ecological design. The content of the restrictions results from the conditions of environmentally sustainable development and ecological safety of the industrial regions. The typical restrictions are the mathematical formulations of the demand of fulfillment of the atmospheric quality standards.

The characteristics and restrictions might be global, distributed, and local. Adjoint problems, methods of inverse modelling, sensitivity and optimisation methods are generated with the help of such functionals. The structure and the principles for construction of the model set for the system of the atmosphere of an industrial region are developed for practical implementation of the proposed concept. In the concept, a region is considered as an element of the climatic system which is both a source and a receptor of pollution.

To combine the models of processes, observational data, and a set of the functionals in the frames of forward and back relations, we suppose that each element may contain uncertainty. In this case, it is naturally to formulate a variational principle for construction of such relations based on minimum conditions for a total measure of all uncertainties. The proposed variational principle ensures the agreed description of all models and processes in physical sense and the construction of the appropriate structure of numerical schemes and algorithms.

The essence of the variational principle is as follows. It is necessary to define the basic sensitivity relations for a chosen set of the functionals in such a way that they should be dependent on parameter variations solely (and not on those of the state functions themselves). The functionals and models may be as linear as nonlinear with respect to the state functions. The bi-stationary conditions for the functionals with respect to the variations of the adjoint functions and the state functions define the mutually agreed structure of numerical schemes for basic and adjoint problems. Each functional generates its own adjoint problem.

Sensitivity relations give the constructive base for establishing direct and inverse connections between the variations of parameters and those of functionals of general type. Arising sensitivity functions (SFs) unite the solutions of forward and adjoint problems. All internal degrees of freedom which are in the models of the processes and in the models of observations are concentrated in SFs. The methods of forward modelling can be applied to a given set of input parameters and data for simulation of the spatial and temporal behavior of the state functions. Then the values of the objective functionals are calculated. It should be noted, that the feedback in these models is usually realized by means of new runs with changed parameters.

The variational methods using the adjoint problems can give the backward propagation of information which is contained in the target functionals, to parameters of models through the SFs. This gives a basis for realization of the feedback algorithms and methods of the control theory. The variational technique in combination with the methods of control, risk, and sensitivity theories has a wide area for applications. In particular, among these applications are the following:

- diagnosis of the model quality,
- uncertainty estimation,
- data assimilation,
- reconstruction of state functions using models and observational data,
- sensitivity studies,
- parameter identification,
- design of measurements,
- ecological prospecting,
- estimation of risk and vulnerability areas,

- problems of “receptor-source” and “source-receptor” types,
- revealing the sources of pollution and estimation of source parameters,
- environmental quality and risk control,
- optimisation of the environmental protection or mitigation strategy.

In the next sections the main points of the concept will be shortly presented.

2.1. Statement of the problem

A rather broad spectrum of environmental protection problems exists. This scientific field unites many disciplines such as physics, chemistry, ecology, biology, economy, mathematics, etc. Here we present the mathematical tool intended to combine diverse knowledge in this interdisciplinary issue. The relevant processes are described by hydrodynamic models of the climatic system, models of transport and transformation of moisture, chemically and optically active pollutants in gas and aerosol phase. To handle the process models and monitoring systems with the purpose of treating the interactions between them both in the forward and inverse modes, we assume that all elements of the system (i.e. models and observations) can contain uncertainties and errors. In this case, it is natural to construct the algorithms for realization of such communications that proceed from conditions of minimization of some total measure of uncertainties and errors.

For the description of processes and their mathematical models we introduce some types of objects such as

- state functions $\boldsymbol{\varphi} = \{\varphi_i(\mathbf{x},t),\ i = \overline{1,n}\} \in Q(D_t)$,
- model parameters $\mathbf{Y} = \{\mathrm{Y_i}(\mathbf{x},\mathrm{t}), \mathrm{i} = 1, \mathrm{n_p}\} \in \mathrm{R}(\mathrm{D_t})$,
- and adjoint functions $\boldsymbol{\varphi}^* = \{\varphi_i^*(\mathbf{x},t),\ i = \overline{1,n_c}\} \in Q^*(D_t),\ n_c \geq n$.

Here $D_t = D \times [0,\bar{t}]$, D is a domain of spatial coordinates $\mathbf{x} = (x_1, x_2, x_3)$, $t \in [0,\bar{t}]$ is a time interval, $Q(D_t)$ is the space of the state functions satisfying the boundary conditions at the boundary Ω_t of the area D_t. The functional space $Q^*(D_t)$ is adjoint to the space of the state functions $Q(D_t)$, $R(D_t)$ is the range of admissible values of parameters. The domain D_t is considered to be in three variants: a sphere, a hemisphere or limited areas on the sphere.

To solve the above mentioned problems, we need to formulate some goal functionals for short description of the generalized characteristics of the state variables of complicated dynamic systems. The form of such functionals is conveniently chosen from the statements of mathematical models of the processes under discussion. Without going into details, let us write a model in which dynamics of the atmosphere as well as transport and transformation of impurities are presented. The structure of such a model can be given in the operator form:

$$L(\boldsymbol{\varphi}) \equiv B\frac{\partial \boldsymbol{\varphi}}{\partial t} + G(\boldsymbol{\varphi}, \mathbf{Y}) - \mathbf{f} - \mathbf{r} = 0, \tag{2.1}$$

$$\boldsymbol{\varphi}^0 = \boldsymbol{\varphi}_0^0 + \boldsymbol{\xi} \quad , \quad \mathbf{Y} = \mathbf{Y}_0 + \boldsymbol{\zeta},$$

where $\boldsymbol{\varphi}(\mathbf{x},t)$ is the state vector that belongs to the real vector space $Q(D_t)$, B is a diagonal matrix, $G(\boldsymbol{\varphi}, \mathbf{Y})$ is a nonlinear matrix differential operator, $\mathbf{f}$ is a source function, The vector $\mathbf{Y}$ describes the model parameters belonging to a range of admissible values of $R(D_t)$, $\boldsymbol{\varphi}^0$ is an initial state, $\boldsymbol{\varphi}_0^0, \mathbf{Y_0}$ are a priori estimates of the corresponding objects. The functions $\mathbf{r}, \boldsymbol{\xi}, \boldsymbol{\zeta}$ describe the errors and uncertainties of the model, initial data and parameters respectively. The boundary conditions depend on the problem formulation. They participate in the definition of the class of functions $Q(D_t)$.

To be more specific, let us consider only those models from (2.1) which are directly describing the processes of heat, moisture, radiation, and pollutants transport and transformation in the atmosphere as follows:

$$L\varphi \equiv \frac{\partial \pi \varphi_i}{\partial t} + \mathrm{div}\pi(\varphi_i \mathrm{u} - \mu_i \mathrm{grad}\,\varphi_i) + \pi((\mathrm{H}\varphi)_i - \mathrm{f}_i(\mathrm{x},\mathrm{t}) - \mathrm{r}_i) = 0, \;\; i = \overline{1,n}. \tag{2.2}$$

Here the components of the state vector φ_i are the potential temperature, the mixing ratios of humidity in the atmosphere (water vapor, cloud water, rain water, snow and ice crystals), the concentration of pollutants in gas and aerosol phase; $\mathbf{f} = \{f_i(\mathbf{x},t)\}$ is the functions of heat, moisture and pollutants sources; $\mathbf{r} = \{r_i\}$ are the functions describing uncertainty and errors of the models; $\mathbf{u} = (u_1, u_2, u_3)$ is the velocity vector; $\boldsymbol{\pi}$ is the function depending on the coordinate system and satisfying the continuity equation in (1); $\mu_i = (\mu_1, \mu_2, \mu_3)_i$ are the diagonal tensor of coefficients of turbulent exchange for a substance φ_i in the coordinate direction $\mathbf{x} = \{x_i\}, i = \overline{1,3}$; $H(\boldsymbol{\varphi})$ is a nonlinear matrix operator which describes the local processes of transformation of the corresponding substances. The functions $\mathbf{u}, \mu_i, f_i$ and input data of initial and boundary conditions are included in vector $\mathbf{Y}$.

To take into account the formation and transformation of aerosols (nucleation, coagulation, condensation, etc.), one more variable, i.e. the size of particles, is introduced. Besides, the additional members having integro-differential structure are added to the operator of transformation.

The processes of dry and wet deposition are considered in the vertical terms of the transport operator. An example of the base cycle of chemical transformation of a multicomponent mixture of pollutants for typical conditions in the atmosphere of industrial regions is presented in (Penenko,Aloyan, 1985).

As it was accepted in (2.1), the initial conditions at $t = 0$, the boundary conditions, and the model parameters in (2.2) can be written in the form:

$$\varphi^0 = \varphi_a^0 + \xi(\mathbf{x}), \;\; (R_b(\varphi))_i - g_i = \varepsilon_i, \;\; i = \overline{1,n}, \;\;\; \mathbf{Y} = \mathbf{Y_a} + \zeta(\mathbf{x},t), \tag{2.3}$$

where φ_a^0 and $\mathbf{Y_a}$ are the set of the prior estimations of the initial fields φ^0 and the vector of parameters $\mathbf{Y}$; $\xi(\mathbf{x})$, $\zeta(\mathbf{x},t)$ are the errors and uncertainties of initial fields and parameters; R_b are the operators of boundary conditions, and g_i, ε_i are functions describing sources and uncertainties at the boundary Ω_t of the domain D_t.To include observational data in the model system it is necessary to formulate a functional dependence between the data of measurements and the state functions in the forward and inverse modes

$$\boldsymbol{\Psi}_m = [\mathbf{W}(\varphi)]_m + \boldsymbol{\eta}(\mathbf{x},t), \tag{2.4}$$

where $\boldsymbol{\Psi}_m$ the set of measured is values; $[\mathbf{W}(\varphi)]_m$ is the set of observational models; $\boldsymbol{\eta}(\mathbf{x},t)$ are the errors and uncertainty of these models and data. The values $\boldsymbol{\Psi}_m$ are defined on the set of points $D_t^m \in D_t$. The symbol $[\,]_m$ denotes the operation of data transfer from D_t to D_t^m. Under observational model we mean a mathematical description of the representation of the measured function in terms of the state functions of the processes model (2.1-2.2).

2.2. The variational formulation of the model of processes

Integration of all models in a united system is carried out by means of variational principles.

Therefore, along with the differential formulation of the problem, we use the variational formulation of the model (Eqs.(2.1) – (2.2))

$$I(\varphi,\mathbf{Y},\varphi^*) = \int_{D_t} (L(\varphi),\varphi^*) dDdt = 0\,, \tag{2.5}$$

where φ^* is sufficiently smooth function from the space $Q^*(D_t)$ adjoint to the space of the state functions $Q(D_t)$.

The integral identity (Eq.2.5) is constructed with the use of boundary and initial conditions. Having executed all necessary transformations in Eq. (2.5) for the model (Eqs. 2.1-2.2), we finally receive integral identity in the form of

$$I(\varphi,\mathbf{Y},\varphi^*) \equiv \sum_{i=1}^{n} \left\{ (\Lambda\varphi,\varphi^*)_i + \int_{D_t} (H(\varphi)_i - f_i - r_i)\varphi_i^* \pi dDdt \right\} = 0\,, \tag{2.6}$$

$$(\Lambda\varphi,\varphi^*)_i \equiv \left\{ \int_{D_t} \left\{ 0.5\left[(\varphi^* \frac{\partial \pi\varphi}{\partial t} - \varphi \frac{\partial \pi\varphi^*}{\partial t}) + (\varphi^* \,\mathbf{div}\, \pi\varphi\mathbf{u} - \varphi\, \mathbf{div}\, \pi\varphi^*\mathbf{u}) \right] + \right.\right.$$

$$\left. \pi\mu\, \mathbf{grad}\, \varphi\, \mathbf{grad}\, \varphi^* \right\} dDdt + \int_{D} 0.5\varphi\,\varphi^* \pi dD \Big|_0^{\bar{t}} + \tag{2.7}$$

$$\left. \int_{\Omega_t} (0.5\varphi u_n - \mu \frac{\partial \varphi}{\partial n})\varphi^* \pi d\Omega dt + \int_{\Omega_t} ((R_b\varphi) - g - \varepsilon)\varphi^* \pi d\Omega dt \right\}_i .$$

u_n is the normal to the boundary component of the velocity vector. The symbol (,) denotes the energy inner product. Discrete approximations of Eqs. (2.5) - (2.6) are constructed in such a way that they should keep the basic properties incorporated in integral identity.

2.3. Variational principles in the problems of environment protection

To formulate the variational principles we introduce a set of functionals which express the generalized characteristics of the processes and mathematical models. For the purposes of monitoring, forecasting, management and designing let us define a set of such characteristics by means of the functionals of a general type

$$\Phi_k(\varphi) = \int_{D_t} F_k(\varphi)\chi_k(\mathrm{x},t) dDdt \equiv \left(F_k(\varphi), \chi_k(\mathrm{x},t)\right), \quad k = 1,...,K,\ K \geq 1\,, \tag{2.8}$$

where $F_k(\varphi)$ are the functions of the given form defined and differentiated on the set of the model state functions $Q(D_t)$, $\chi_k(\mathrm{x},t) \geq 0$ are the weight functions, $\chi_k \in Q^*(D_t)$ and $\chi_k(\mathrm{x},t)dDdt$ are the corresponding measures of Radon and Dirac in D_t^h (Schwartz, 1967). At a suitable choice of the functions $F_k(\varphi)$ and $\chi_k(\mathrm{x},t)dDdt$ in Eq. (2.8) by means of the functionals of this type, it is possible to describe the various generalized global, distributed and local characteristics of the system behavior, as well as the ecological restrictions on the environment quality, the results of observations of various types, the criteria of management and designing, the criteria of model quality etc (Penenko, 1994. Penenko and Tsvetova, 2004).
“Quality” functionals help us to include the data of observations (Eq.2. 4) to the modelling system for goals of data assimilation and parameter identification. Usually they are defined as an estimation of a measure of all uncertainties in the structure of Eq. (2.4)

$$\Phi_0(\varphi) = \left((\Psi_m - [\mathbf{W}(\varphi)]_m)^T \chi_0 \mathbf{S} (\Psi_m - [\mathbf{W}(\varphi)]_m) \right)_{D_t^m} \equiv (\eta^T M_1 \eta)_{D_t^m} \quad , \tag{2.9}$$

where index T denotes the transposing, $\mathbf{S}$ and $M_1 = \chi_0 S$ are weight matrices for formation of scalar product on the set of the observed data of the various nature. They are the positive definite Hermitian matrix, χ_0 is the weight function defining a configuration of the space-time support of observations D_t^m in D_t and a measure for representation of Eq. (2.9) in the form of Eq.(2.8). The main property of the functionals of the type (2.9) which makes them appropriate for control problems and data assimilation, that they describe the norm of residuals (“principle of residuals”).
To locate the sources and design observations in addition to the functionals of Eq. (2.9), it is necessary to introduce the sequence of the functionals of the type of Eq. (2.8). Each of them describes the individual observation in the structure of Eq. (2.4).
The functionals of the following types are introduced for the solution to the problems of optimisation of nature protection activity, control of environmental quality and ecological designing in the presence of constrains. Using the definition (Eq. 2.8), we write down them both as equalities and inequalities

$$\Phi_{ri}(\varphi) = \int_{D_t} F_{ri}(\varphi) \chi_{ri}(\mathrm{x}, t) dDdt \le 0, \quad i = \overline{1, n_c} \ , \tag{2.10}$$

where functions $F_{ri}(\varphi)$ are defined in such a way that all the integrated, local, and distributed restrictions on the state functions could be accounted by means of Eq. (2.10), n_c is the total number of restrictions. In particular, the equality in Eq. (2.9) takes place when it is necessary to consider the restrictions in the form of inequalities distributed in D_t

$$\psi_i(\varphi, \mathbf{x}, t) \le 0, \quad i = \overline{1, n_\psi} \ , \tag{2.11}$$

where $\psi_i(\varphi, \mathbf{x}, t)$ are continuous and, in general, nonlinear functions, n_ψ is the number of these inequalities. Due to high dimension of the problems the direct inclusion of distributed inequalities into the algorithms offers the principle difficulties. To overcome them, the local constraints (Eq.2.11) are transformed to the equivalent integral form of Eq. (2.9) with the strict equality to 0. This may be distinguished by choosing F_{ri} in the form

$$F_{ri} = \left| |\psi_i| + \psi_i \right|.$$

In such a way, all the distributed constraints are involved into the general scheme of variational principles and sensitivity methods with the use of adjoint problems regardless of the state function dimension (Penenko,1994).
For convenience of the algorithm construction, all functionals of Eqs. (2.8) - (2.10) are formed by the same principle as inner product, i.e. they are written in the form of global integrals on the domain D_t with the integrand expressions defined in the space of the state functions and with non-negative weight functions taken from the corresponding adjoint spaces. From the variational principle point of view numerical models are considered as the constraints on the class of functions and as connections between parameters and the state functions.
Thus, the basic set of concepts and base elements of the modelling system are defined. Now it is possible to formulate a variational principle to link all elements and algorithms in a uniform system.
The essence of variational principle is expressed as follows. It is necessary to define the basic sensitivity relations for the chosen set of functionals to the variations of input parameters of the models and external forcing so that they would be independent on the first order variations of the state functions, adjoint functions, and functions of uncertainty of corresponding objects. The

functionals and models can be both linear and nonlinear with respect to the state functions. However, while parameters (including sources) are varied, the estimations of the functionals should always be stationary in relation to the first order variations of the state functions, adjoint functions, and functions of uncertainty of the corresponding objects. The conditions of such stationary state define mutually co-ordinated structure of numerical schemes for the basic models and the adjoint problems generated by the variational principle.
It is convenient to generate all algorithms for realization of variational principle on the basis of the set of extended functionals which unite the functionals and models in the discrete form (Penenko,1981)

$$\tilde{\Phi}_k^h(\varphi) = \Phi_k^h(\varphi) + \mathbf{I}^h(\varphi, \mathbf{Y}, \varphi^*), \; k = \overline{1,K}, \; K \ge 1, \tag{2.12}$$

where the index h denotes discrete analogs. Discretization of all functionals is made with the use of weak approximation, splitting, and decomposition methods. To obtain the splitting schemes, the integrals in time are approximated by the cubature formulas within the fractional steps. The different parts of the general operator are taken at the separate fractional steps. The cubature formulas for all objects are harmonized in the discrete analogues of the functional spaces.
The usage of the variational principles for the approximation of the integral identity and the extended functionals in combination with decomposition and splitting methods, allows us to present the complex, multidimensional problems as a set of one-dimensional subproblems.
The formulated variational principle has universal character. Its concrete content is defined by the set of functionals and variational formulations of models in the form of the augmented functionals (Eq.2.12).

2.4. Universal algorithm of forward and inverse modelling

To formulate the statements of inverse problems and to construct the algorithms for their solution we take advantage of optimisation theory and techniques of variational calculus. The main functional for organisation of modelling system is formulated by analogy with Eq. (2.12) in such a way that all models and the accessible data considered in it, as well as the influence of uncertainties being in them, are minimized

$$\begin{aligned}\tilde{\boldsymbol{\Phi}}_k^h(\boldsymbol{\varphi}, \boldsymbol{\varphi}^*, \mathbf{Y}, \boldsymbol{\eta}, \mathbf{r}, \boldsymbol{\xi}, \boldsymbol{\zeta}) &= \boldsymbol{\alpha}_0 \boldsymbol{\Phi}_k^h(\boldsymbol{\varphi}) + 0.5\Big\{\boldsymbol{\alpha}_1(\boldsymbol{\eta}^T M_1 \boldsymbol{\eta})_{D_t^m} + \boldsymbol{\alpha}_2(\mathbf{r}^T M_2 \mathbf{r})_{D_t^h} \\ &+ \boldsymbol{\alpha}_3(\xi^T M_3 \xi)_{D^h} + \boldsymbol{\alpha}_4(\zeta^T M_4 \zeta)_{R^h(D_t^h)}\Big\}^h + \left[I^h(\varphi, Y, \varphi^*)\right]_{D_t^h}.\end{aligned} \tag{2.13}$$

Here the first term represents the target functional of the type of Eq. (2.8), the four following members express, in total, a measure of uncertainties of the model of observations, the models of processes, initial data and parameters, accordingly. They are constructed by analogy with (2.9). We remind that all input parameters of models and sources of external influences are included in the vector $\mathbf{Y}$. The last term contains the description of numerical model in variational formulation. $\mathbf{M}_i, i = \overline{1,4}$ are the positive definite weight matrixes. $\alpha_i, i = \overline{0,4}$ are parameters given to describe the structure of the algorithm. The discrete analogs of the functionals (Eqs.2.12-2.13) are constructed with the use of weak approximation, splitting, and decomposition. Finally, the discrete approximations of models and algorithms for modelling are obtained from the stationary conditions for the extended functionals $\tilde{\boldsymbol{\Phi}}_k^h$ to the variations of different components.

The scheme of algorithm constructions consists of the following items:

(1) The approximations for the main problems and methods of forward modelling are produced from the stationary conditions for the functionals $\tilde{\boldsymbol{\Phi}}_k^h$ to the variations of the adjoint function components:

$$\partial\tilde{\Phi}_k^h / \partial\varphi^* = 0 .$$

(**2**) The adjoint problems and inverse modelling approximations can be obtained from the stationary conditions for the functionals $\tilde{\Phi}_k^h$ to the variations of the state function components

$$\left\{\partial\tilde{\Phi}_k^h / \partial\varphi = 0,\ \varphi_k^*(x)\big|_{t=\bar{t}} = 0\right\}.$$

(**3**) If uncertainty is present in the model, then the stationary conditions to the variations of the components of these functions give the system of equations for uncertainty estimations with the help of measured data incorporated in the functionals (Eq. 2.12) through the corresponding sensitivity functions (SF):

$$\partial\tilde{\Phi}_k^h / \partial\mathbf{U} = 0 ,$$

where $\mathbf{U} = \{\mathbf{r}, \xi, \zeta, \varepsilon\}$ is an uncertainty function.

(**4**) The stationary conditions to the variations of model parameters, including sources of external influences, lead to the system of the equations for finding these parameters with the use of actual information. In essence, these are the algorithms of feedback realization from the functionals to the model parameters using the SFs:

$$\Gamma_k = \partial I^h(\varphi, \mathrm{Y}, \varphi_k^*) / \partial\mathbf{Y} \ \text{ or } \ \Gamma_k = \partial\tilde{\Phi}_k^h / \partial\mathbf{Y} .$$

The operations of differentiation in items (**1**)-(**4**) are carried out for each of grid components of the state functions, the adjoint functions, and parameters. Structurally they are realized by means of Gateaux derivatives for the functionals of Eqs. (2.12)-(2.13) with respect to each of their functional arguments.
The system obtained is the central kernel of the computing technology for forward and inverse modelling for the risk and control problems.

2.5. Sensitivity studies

The relations between the variations $\delta\Phi_k^h(\varphi)$ and the variations of model parameters are described by the sensitivity relations and realized by means of SFs. Their expressions are defined by the coefficients at the variations of the corresponding parameters in the basic sensitivity relation for $\tilde{\Phi}_k^h(\varphi)$ written according to three stationary conditions specified above

$$\delta\Phi_k^h(\varphi) \equiv \frac{\partial}{\partial\alpha} I^h(\varphi, \boldsymbol{Y} + \alpha\ \delta\boldsymbol{Y},\ \varphi_k^*)\big|_{\alpha=0} \equiv (\boldsymbol{\Gamma}_k, \delta\boldsymbol{Y}) \equiv \sum_{i=1}^{N} \Gamma_{ki}\delta\boldsymbol{Y}_i . \tag{2.14}$$

Here α is a real parameter, $\boldsymbol{\delta}\mathbf{Y}$ is a vector of parameter variations, φ is the solution of the direct problem(item **1**), φ_k^* is the solution of the adjoint problem (item **2**) corresponding to the functional $\Phi_k^h(\varphi)$. The algorithms for the construction of the basic sensitivity relations and SFs for the problems of the considered class are described in (Penenko,1981,1994, Penenko and Tsvetova,1999).
The equations of a feedback are produced after the calculation of the sensitivity relations (Eq.14) for all functionals of Eqs. (2.8), (2.10) participating in the statements of the problem. Starting from the methods of control theory and following (Penenko,1981,1994) , we put down these equations in the form

$$\frac{\partial\mathbf{Y}}{\partial t} = -\aleph\boldsymbol{\Gamma}_k , \tag{2.15}$$

where Γ_k are the SFs for target functionals, and $\aleph$ is a coefficient of proportionality. The correction of the right hand side of Eq. (2.15) is made if the restriction functionals (Eq. 2.9) are present. The gradient projection method is used for these purposes.
The most important fact in this consideration is that the relations (2.14) are the evidence for the interrelation of all elements of the models. The solutions of the direct and adjoint problems take to themselves all inner degrees of freedom in the models. As a result, the terms with variations of parameters and forcings solely need for assessment of the goal functional changes.
It should be noted that in dependence of the aims of the study and for convenient interpretations, sensitivity functions are referred as influence, danger, risk, vulnerability, informativity observability, etc. functions.

2.6. The algorithms for risk assessment

Assessment of environmental risk and vulnerability of territories with respect to anthropogenic effects is one of the typical problems of environmental prognosis and design. From ecological point of view, each industrial source, even in normal conditions, has an influence on the environment. The fact itself that a source falls into the sensitivity region for the goal or restriction functional, already says about the risk to obtain the pollution from it in the receptor zone. The appearance of the toxic products as the result of primary substances transformation testifies to risk, too. Therefore the sensitivity relations which are a measure of direct influence of the source variations and transformation mechanisms on the value of functional variation (the influence of the source itself, in the linear case); give the algorithms for quantitative estimates of the risk/vulnerability domains and for revealing the sources of this risk.
The methods of sensitivity theory can be directly used for estimation of ecological risks and vulnerability of territories in relation to the influence of anthropogenic factors considered in the models of processes, such as the changes of heat sources, moisture, air quality and changes of the Earth surface characteristics.
The sensitivity functions are calculated through the solutions of the main and adjoint problems for the model with undisturbed values of input data. And consequently, they have the deterministic character. But the variations of parameters, initial and boundary conditions and sources may be both deterministic and stochastic.
For a quantitative estimation of ecological risks we introduce some threshold values for functional variations (Eq.2.14). Let us denote them as $\Delta_k^s, \quad k = \overline{1, K}$. Then, the situations may be considered as conditionally ecologically safe if the following inequalities are true for them

$$\left|\delta\Phi_k\right| \le \Delta_k^s \ . \tag{2.16}$$

Otherwise, the situations may be classified as that of ecological risk. It follows from Eq. (2.14), that the check of the inequalities of "ecological well-being" (Eq. 2.16) does not cause the difficulties if the sensitivity functions and quantitative information on variations of parameters are available. In case of the deterministic variations of sources and parameters, the estimation of magnitude of functional variations can be calculated by formulas

$$\left|\delta\Phi_k\right| \le \sum_{i=1}^{N} \left|\Gamma_{ki}\right| \left|\delta Y_i\right| \ . \tag{2.17}$$

Using these estimations together with inequalities of Eq. (2.16) it is possible to make the direct conclusion whether the situation refers to a category of well-being or risk.
If variations of parameters and sources are random, the estimations become more complicated as compared to the deterministic case, since it is necessary to work with multidimensional spaces of SFs and parameters with stochastic disturbances. Consider one of approaches to obtaining the

needed assessments in the deterministic-stochastic case based on the methods of sensitivity theory (Penenko,1981) and the mathematical risk theory (Grandle,1992).
Two methods are commonly used in practice to describe variations. The first one consists in the following. Based on *a priory* information on the character of a parameter or a source, some form of the distribution law for variations is postulated and, accordingly, some parameters needed to match the supposed distribution with actual one are specified. The normal distribution is used most often, because most actual distributions are close to the normal one and the normal law is convenient for solution of different problems.
In the second case, the first two moments of the multidimensional distribution law (mathematical expectation and covariance matrix) are specified, but the law itself is not always specified. The both methods are similar, because the normal law is completely determined by the mathematical expectation and the covariance matrix. The second method in more general. The results it gives are valid for any, not necessarily normal, distribution of variations with the given characteristics.
Denote the mathematical expectations and the covariance matrix of the vector $\delta\mathbf{Y}$ as $\mathrm{E}(\delta Y)$ and $\mathrm{D}(\delta\mathbf{Y})$, respectively. The $N\times N$ covariance matrix $\mathrm{D}(\delta\mathbf{Y})$ is nonnegative definite. It has a block structure matched with the structure of the vector $\delta\mathbf{Y}$. If some components of $\delta\mathbf{Y}$ are uncorrelated, the appropriate blocks of $\mathrm{D}(\delta\mathbf{Y})$ are diagonal, while full blocks of $\mathrm{D}(\delta\mathbf{Y})$ correspond to the correlated components of $\delta\mathbf{Y}$.
The vector $\mathbf{\Gamma}_k$ depends on undisturbed values of parameters and the state vector. Therefore , for particular situations it can be thought non-random. Taking into account the properties of mathematical expectation and covariance matrices at linear transformations of random vectors, we obtain the following estimates for mathematical expectations $\mathrm{E}(\delta\Phi)$ of variations of the functional $\delta\Phi$:

$$\mathrm{E}(\delta\Phi)=\sum_{i=1}^{N}\Gamma_i\mathrm{E}(\delta Y_i) \tag{2.18}$$

and for the variance $\mathrm{D}(\delta\Phi)$

$$\mathrm{D}(\delta\Phi)=(\mathrm{D}(\delta\mathbf{Y})\mathbf{\Gamma},\mathbf{\Gamma})\,. \tag{2.19}$$

Hereinafter the number index in the functional is omitted. Thus, the variance is determined through a square form of the covariance matrix of the variation vector and the vector, whose components coincide, in view of Eq.(2.14), with the sensitivity functions of this functional. It is obvious that $\mathrm{D}(\delta\Phi)$ in nonnegative. The scalar product in Eq.(2.19) is introduces by analogy with Eq.(2.14), as in a finite-dimensional vector space.
In the particular case, when errors in the components of $\delta\mathbf{Y}$ are uncorrelated, the covariance matrix is diagonal and Eq.(2.19) has the simplest form

$$D(\delta\Phi)=\sum_{i=1}^{N}\Gamma_i^2 D_i\,. \tag{2.20}$$

Note that in Eqs.(2.18)-(2.20) the sum includes only those terms, in which the sensitivity function is larger than some threshold.
According to Eq.(2.14), variations of $\delta\Phi$ is determined as a linear combination of random parameters. If N is quite large and all components of $\delta\mathbf{Y}$ do not differ largely from the normal distribution, then, based on the central limit theorem of the probability theory, we can assume that the distribution law for $\delta\Phi$ tends to the normal one.
The assumption of the normal distribution law considerably facilitates the problem, because to characterize this distribution completely , it is sufficient to know its mathematical expectation and the variance or the corresponding covariance matrix.
Using the values of $\mathrm{E}(\delta\Phi)$ and $\mathrm{D}(\delta\Phi)$ and the assumption of the normal distribution of $\delta\Phi$ as a random function, we can obtain some estimates of $\Phi(\varphi)$. The technique for constructing these

estimates is rather well-developed now. In its consideration we follow (Penenko,1981).
The probability that the value of $\delta\Phi$ falls in a given region Δ (i.e., $|\delta\Phi| \le \Delta$) is determined as

$$P(\delta\Phi \le \Delta) = \int_{\Delta} f(x)dx, \quad x \equiv \delta\Phi\,, \tag{2.21}$$

where $f(x)$ is the probability density function (pdf) of the distribution of x:

$$f(x) = e^{-(x-\mathrm{E}(x))^2/2\mathrm{D}(x)} / \sqrt{2\pi \mathrm{D}(x)}, \tag{2.22}$$

and $\mathrm{E}(\delta\Phi)$ and $\mathrm{D}(\delta\Phi)$ are determined by Eqs (2.18),(2.19),or (2.20). The integral is taken over the region $(-\Delta \le x \le \Delta)$. The probabilities of the fulfillment of the inequalities (2.16) expressing the conditions for the situation under analysis are of interest to be categorize as ecologically safe:

$$R^s = P(|\delta\Phi| \le \Delta^s)\,. \tag{2.23}$$

Assuming the normal distribution law for $\delta\Phi$ with pdf (2.22), we have for the sought probabilities

$$R^s = \frac{1}{\sqrt{2\pi \mathrm{D}(x)}} \int_0^{\Delta^s} e^{-(x-\mathrm{E}(x))^2/2\mathrm{D}(x)} dx = \frac{1}{\sqrt{2\pi}} \int_0^{\lambda} e^{-t^2/2} dt = \Psi(\lambda), \tag{2.24}$$

where $\lambda = \lambda(R^s) = \left[\Delta^s - E(x)\right] / \sqrt{D(x)}$, $\Psi(\lambda)$ is the probability integral. The probability that the situation is categorized as ecologically hazardous R^r is estimate as

$$R^r = 1 - R^s \equiv P\left\{\delta\Phi > \Delta^s\right\}.$$

On the other hand, if we specified a certain acceptable level of safety probability R^s, then, based on it, we can determine λ from Eq. (2.23) and estimate the safety range

$$\left|\Delta^s - \mathrm{E}(\delta\Phi)\right| = \lambda \sqrt{\mathrm{D}(\delta\Phi)}\,.$$

In the problem of ecological designing, in addition to assessment of a situation as a whole, it is necessary to consider the worst possible cases for the atmospheric quality in some receptor region. For this purpose, zones of local maxima of the sensitivity function and zones of the location of potentially high-power sources (in respect to pollutant emission) are being sought. If these zones coincide, situations of high ecological risk/vulnerability can occur. In such cases more thorough investigation is necessary, for example, initiation of direct modeling scenarios with a given set of sources and various versions of emissions.

2.7. The algorithms for risk control

Risk control is a key element for the choice of strategy of sustainable development and social safety. The main objectives are development of a concept and a methodology of optimisation of risk control in accordance with the given criteria and restrictions as well as elaboration of express-methods for assessment of tendencies of increasing or decreasing risks for chosen region-receptors undergone the influence of different factors.
The proposed methodology is based on a variational principle, optimisation methods and sensitivity theory applied to the models of transport and transformation of substances, heat and humidity. The goal functionals for control strategy forming are chosen with allowance of the requirements of

multi-disciplinary expertise. The functionals may describe, for example, cost of damage, cost of management, technological improvements, the costs of protecting or recovering health, etc.
All functionals and restrictions containing the state functions are described by an integral form which is dictated by the variational principle for construction of the adjoint problems and sensitivity functions. The control algorithms are realized by the combination of the forward and inverse modelling techniques.
Optimisation models are referred to the interactive tools. Generally speaking, their realization does not avoid the iterations. This is mainly due to the fact that the system has a large number of freedom degrees, which are managed only by iterations in the interactive regime.

Let us describe the main stages of the system organisation of the algorithms:

- the set of goal functionals and restrictions is prescribed;
- the set of receptors is prescribed and the structure of the functionals for their description are defined;
- sensitivity relations are constructed and calculate (to this moment, we need the solutions of the forward and adjoint problems for chosen system of functionals)
- the regions of risk/vulnerability are revealed from the sensitivity analysis for given set of receptors and functionals;
- the sources being in the region of risk/vulnerability are defined;
- the sources are ranged with respect to the potential danger and the SFs' significance levels in the zones of sources localization;
- the sources are separated into two groups: accessible to control or not (e.g., if the source is abroad)
- the control strategies are designed by means of the feedback equations;
- examination of criteria and restrictions after the strategy was applied;
- in case of need, the parameters are corrected and the process is repeated beginning with the third item.

It should be noted, if a priory data on location of the sources are known then the control problem does not meet principle difficulties. The other case if location of sources and time of release are unknown. The revealing of such objects is a nontrivial problem. In this case, a priory information about the specific character of the releases (radioactivity, for example) makes the searching slightly easier. In general case, the problems of such type have to be solved together with the observation planning. This allows the region of searching to be narrowed by taking into account the additionally measured data. For express-analysis of tendencies, a simplified scheme is proposed. It is just the part of the general scheme and is limited to the solution of the source-receptor and receptor-source problems taken with the parameters estimated on a priory data without iterations.

2.8. The advantage of variational approach

The advantages of variational methods with adjoint problems in environmental studies are in the following. First, they have a flexible structure which can be easily adjusted to various mathematical models. Secondly, they are also conveniently adapted to sets of functionals and restrictions, as well as to different means of data assimilation. The variational technique gives the possibility to incorporate a priori knowledge into the modelling technology with the help of the special functionals. Moreover, if splitting and decomposition methods are used, the algorithms of simple structure and effective realization can be obtained. They are easily co-ordinated at different stages of the solution of the problem in the forward (direct) and adjoint (inverse) modes.
The methods of the control and optimisation theories have actively been developed in different areas of science and technology during the last four decades. From the mathematical point of view

they are of variational nature. As a consequence, the methods of the sensitivity theory generated from variational principles give a powerful formalism for estimating the variations of functionals of general form and particularly for evaluating risks and vulnerability of territories with respect to disturbances of acting factors in the models.
Using modern computing resources and technologies, the adjoint variational algorithms can effectively be realized at relatively reduced computational cost. Usually, one cycle of simulation includes the integration of forward and inverse models. The additional cost of inverse runs for sensitivity studies for one functional or for an ensemble of functionals, that generate just one adjoint problem, is approximately equal to the cost of the forward model run. If we need to calculate the SFs with respect to parameter variations, the additional cost of each SF is proportional to the dimension of the space-time grid domain. The total cost is obtained as the sum of the partial SF's costs over the number of parameters.
In new methods of data assimilation using splitting and decomposition techniques (Penenko and Tsvetova, 2002, Penenko A.,2006), the cost of one cycle of assimilation is proportional to the cost of the run for sensitivity studies of quality functionals. As regards the control and optimisation algorithms, the cost depends on the formulation of the problem and the approach used for its solution. For the adjoint-based gradient method using of the sensitivity relations, the cost of one iteration cycle is equivalent to the required computational costs of sensitivity relations for all target functionals and constraints defining the task formulation.
Note that optimisation and identification of parameters and sources belong to the class of inverse and ill-posed problems. This requires increased quality of the numerical approximations of the models and algorithms used for forward and inverse modelling. From this point of view, the application of the variational principle with the functionals (2.13) taking the uncertainties into account allows one to regularize the computational algorithms for ill-posed problems in the inverse modelling and data assimilation (Penenko, 2008).
One more important fact should be mentioned here. The matter is in often incorrect use of numerical schemes with flux correction or artificial monotonizators. Such operations are inherent in the commonly used numerical schemes of Harten (TVD), Smolarkevich , Bott , Van Leer and the others. It is known that the artificial monopolization procedures generate non-linear effects of self-limiting diffusion that are non-proper, for instance, for the real pollution transport processes. The reason is that **own** self-limiting diffusion may be generated for **each** particular constituent. As a consequence, this may distort the true evolution of their joint behavior. As a result, the transformation operator gets inconsistent information to define the air quality. For solution of inverse problems with the use of adjoint equations and in adjoint sensitivity analysis the demand of consistency is even stronger.
The variational approach applied for the construction of the numerical schemes of advection-diffusion-reaction operators allows us to obtain **optimal** numerical approximations for the realization of the models in forward and adjoint modes. In particular, a new method of discrete-analytical approximations is developed in (Penenko and Tsvetova, 2008b). It results in schemes possessing the properties of absolute stability, monotonicity, and transportivity. The advantage of the approach is that the discrete-analytical methods maintain the above mentioned properties due to the analytical solutions of the local adjoint problems that use the parameters of the carrying flow **only**. Owing to analytical solutions, the artificial numerical diffusion is avoided in the schemes.

3. Organization and Implementation of Environmental Models

3.1. Atmospheric pollution modelling general aspects

The processes of interest are described by the models of hydrodynamics in the climatic system, the models of transport and transformation of humidity, chemically and optically active pollutants in gaseous state and aerosols. In general sense the main components of environment models usually are:

1. a hydrodynamics component that calculates pressure, three components of wind velocity vector and components of the hydrological cycle;
2. a transport and diffusion component that calculates the three-dimensional motion of gases and aerosols in a gridded model domain;
3. a gas-phase chemistry component that calculates the change in gaseous concentrations due to chemical transformations;
4. an aerosol component that calculates the size distribution and chemical composition of aerosols due to chemical and physical transformations;
5. a cloud/fog component that calculates the physical characteristics of clouds and fog based on information from the meteorological model (or from observation);
6. a cloud/fog chemistry component that calculates the change in chemical concentrations in clouds and fog;
7. a wet deposition component that calculates the rates of deposition due to precipitation (and, possibly, cloud impaction and fog settling) and the corresponding change in chemical concentrations;
8. a dry deposition component that calculates the rates of dry deposition for gases and aerosols and the corresponding changes in their concentrations.

The spatial distribution of meteorological and chemical variables is approximated by three-dimensional gridded systems. The meteorological and the air quality models may have different grid structures over the same domain and methods of the numerical discretization. The detailed modular formation varies from model to model.

The quality of the air pollution modelling/forecast and the Air Quality Information and Forecasting Systems (AQIFS) critically depends on:

(i) the mapping of emissions,

(ii) the air pollution (APM) and chemical transport (CTM) models, and

(iii) the meteorological fields over the considered areas.

The main problem in forecasting air quality is the prediction of episodes with high pollutant concentration in urban or complex geographical condition areas where most of the well-known methods and models, based on in-situ meteorological measurements, fail to realistically produce the meteorological input fields for the urban air pollution (UAP) models. An additional challenge for contemporary AQ models lies in the fact that the legislation on AQ targets to new categories of information, like the likelihood of hot-spot occurrence, or the number of exceedances within a year, that associate AQ forecasting capabilities with urban environment modelling demands, thus making the forecasting issue more complicated.

3.2. Forecasting systems and urban air quality information

About 70% of the European and Russian populations live in cities. A major share of anthropogenic sources of pollutants originated from conurbations. These pollutants have not only local effects (on human health, material, ecosystem), but may impact all the way to the regional (acidification, euthrophication) and global scales (atmospheric composition, climate changes). Urban areas present a challenge to atmospheric scientists, both from the experimentalist and modeler point of view as typically urban areas have high roughness elements penetrating well above the surface layer, heterogeneous distribution of surface features with wide variation in surface fluxes of heat, moisture, momentum and pollutants. Additionally the structure of the conurbation may trigger local meteorological circulations and processes (e.g., heat island, enhanced production of condensation nuclei) as well as enhanced vertical motions resulting in longer residence time of atmospheric compounds. As model resolution is increasing towards a few kilometers or finer and various stakeholders and the public are expecting better targeted meteorological forecasts and products, it has become a necessity to be able to account for, describe and simulate urban effects and processes in various meteorological and air pollution models. On the other hand, this has brought new requirements for observations and measuring strategy in order to be able to describe, simulate and forecast meteorological and concentration fields in urban areas. Integration of these aspects will greatly benefit the development of urban air quality information and forecasting systems (UAQIFS) for a variety of applications and end-users.

Modern numerical weather prediction (NWP) and meso-meteorological models (MetM) able to resolve urban-scale processes are considered to be the main tools in future urban air pollution (UAP) forecasting and assessments because they allow for sufficiently high spatial and temporal resolution and can trace back the linkages between sources and impacts. The Cluster of European Urban Air Quality Research (CLEAR) considers improvements of meteorological data and models for urban areas as one of the targets, because most of the CLEAR projects (FUMAPEX, OSCAR, SAPPHIRE, URBAN AEROSOL, URBAN EXPOSURE, BOND, NEPAP, AIR4EU) need urban meteorological fields for their air quality studies (Baklanov et al., 2006; Sokhi and Baklanov, 2007). However, only the FUMAPEX project (Baklanov, 2006) focuses on the evaluation and improvement of meteorological modelling and pre-processing specifically for urban areas. This work is a logical continuation of the COST Action 715 (Fisher et al., 2005).

3.3. On physical content of typical environmental models

The following urban features can influence the atmospheric flow, microclimate, turbulence regime and, consequently, the transport, dispersion, and deposition of atmospheric pollutants within urban areas:

(1) local-scale non-homogeneities, sharp changes of roughness and heat fluxes,
(2) the building effect in reducing wind velocity,
(3) redistribution of eddies, from large to small, due to buildings,
(4) trapping of radiation in street canyons,
(5) effect of urban soil structure on diffusivities of heat and water vapor,
(6) anthropogenic heat fluxes, including the urban heat island effect,
(7) urban internal boundary layers and the urban mixing height (MH),
(8) different gas and particle deposition efficiencies for different types of the urban surfaces (walls, roofs, streets, etc.),
(9) effects of pollutants (including aerosols) on urban meteorology and climate,
(10) urban effects on clouds and precipitation.

Accordingly the following aspects of urban effects were considered by the FUMAPEX project in improved urban-scale NWP and meteorological models: higher spatial grid resolution and model downscaling, improved physiographic data and land-use classification, calculation of effective urban roughness and urban heat fluxes, urban canopy and soil sub-models, MH in urban areas.

In CARMEN complex (ICMMG), the different aspects of man-made influence are directly taken into account in the models by means of parametrical description of the sources of heat, humidity, pollutants, as well as of the land use categories. The models of transport of substances are considered both in Eulerian and Lagrangian forms in forward and adjoint modes (Penenko and Tsvetova, 1999; Penenko and Baklanov, 2001). For these models, efficient numerical schemes possessing by the properties of stability, monotonicity, and transportivity have been developed. These schemes are adaptive on the accuracy criteria and follow the intensity of the modelling processes. Hydrological cycle describes transport and transformation of humidity in five-component approximation: water vapor, cloud and rain water, ice and snow.

3.4. On-line chemical modelling

In general, the quality of the atmospheric environment in cities is related to at least the following factors: air pollution, urban climate, meteorological conditions and population exposure. It is reasonable to consider them together due to the following reasons:

(i) meteorology is the main source of uncertainty in UAP and emergency preparedness models,

(ii) complex and combined effects of meteorological and pollution components on human health (for example, in France in the hot summer 2003 with a large number of mortality cases),

(iii) effects of pollutants/aerosols on urban climate and meteorological events (such as precipitation and thunderstorms).

Quantification of the combined effect of bio-meteorological factors together with the effects of air pollution is also a major issue. In this context two levels of the integration strategy are considered in the paper:

1. Off-line integration of Urban Meteorology, Air Pollution and Population Exposure models for urban air pollution forecast and emergency preparedness, which is the main issue e.g. in the EC FUMAPEX project (Baklanov et al., 2006).
2. On-line integration of meso-scale meteorological models and atmospheric aerosol & chemical transport models with consideration of the feedbacks of air pollution (e.g. urban aerosols) on meteorological processes and urban climate. This direction is developed by several research organizations (e.g., Grell et al., 2005) and considered in the new COST Action 728 (Sokhi et al., 2005). This will lead to a new generation of models for “chemical weather forecasting”, a goal that is being investigated via the COST action ES0602 (http://www.chemicalweather.eu/).

One example of the on-line integrated MetM-CTM systems - Enviro-HIRLAM - is developing by DMI (Chenevecz et al., 2004; Baklanov et al., 2008; Korsholm et al., 2008). Recently they have developed a new version of the meteorological model HIRLAM with on-line integrated tracer and have implemented a versatile aerosol-cloud module and heterogeneous chemistry in their Atmospheric Chemical Transport Model (Gross and Baklanov, 2004).

Since 1983, numerical methods for transport and transformation of substances - jointly with atmospheric hydrodynamics - have been developed in ICMMG. In dependence on the goal of a study, on-line and off-line coupling has been used. Off-line methods are fitted more often for risk/vulnerability assessment for a long time. On-line technology is more acceptable for meso-climate and atmospheric quality problems. Description of the chemical transformation operators in CARMEN complex is made by different ways including the computer-aided system for construction of kinetic atmospheric chemistry models. A typical for the Siberian conditions atmospheric chemistry cycle of transformation is firstly realized in 1984 (54 components in 276 equations). (Penenko, Aloyan, Bazhin, Skubnevskaya, 1984). To describe aerosols generation and their transformation, additional variable – size of particles – is introduced. The number of size intervals is parametrically given.

The following aspects in development of integrated models are very important in this respect:

1. Testing the quality of operational NWP systems for AQ modelling in urban areas,
2. Improvement of parameterization of urban atmospheric processes and urban physiographic data classification,
3. Development of meteo-processor and interface between urban scale NWP and UAP models,
4. On-line integrated MetM-CTM systems for urban and meso-scale,

3.5. The interaction between air quality modelling and health risk assessment

The quantitative analysis of risks is important to reveal and identify the permitted levels of chemical, biological, radioactive agents/pollutants and etc. in the atmospheric environment and for population as well as change of climatic conditions for population‘s protection. In the air quality modelling for risk assessments there is an increased interest to quantitative methods of analysis of environmental processes in combination with cost and effective methods and methods from a point of view of economic and social development. These methods are required for analysis of environment quality, and they are connected with problems of population health. The interest is also related to methods of comparative analysis, strategy to reduce risks and expenses for practical realization of such approaches. It is important for the comparative analysis of management strategy of the current behavior of environment in order to reach the final aims and in the quantitative estimates of cumulative risks. These depend on the individual pollutants with multiple ways of impact on the environment and population health, and joint influence of multiple effects (Ebel and Davitashvili, 2006).

The problem to formulate such general metrics as well as targeted applications will require additional studies which should be done in collaboration with multidisciplinary specialists. Moreover, such studies need to be done in parallel and in cooperation with research in development of mathematical models and methods of their realization required to achieve the optimal estimates of air pollutant concentrations.

Several approaches are considered for the tasks of risk assessment and control theory:

- Methods of forward modelling based on analysis of ensembles of scenarios for different variants of input data and existing factors. These methods can be implemented with deterministic and stochastic (for example, Monte-Carlo method) algorithms.
- Methods using the adjoint equations generated for evaluation of linear functions such as scalar inner products defined in spaces of both the state functions of models and the weight functions.
- Variational methods for linear and non-linear dynamical systems and functions in combination with methods of the control theory, risk theory, and sensitivity theory. These methods can be realized using a combination of the forward and inverse modelling approaches taking into account the uncertainties of models, parameters, and observational data.

3.6. Scales of the processes/models and scale-interaction aspects

One of the important needs of air quality modelling is to develop further integrated modelling systems that can be used to understand the impacts from aerosols and gas-phase compounds emitted from urban sources at/on the regional and global climate.

Anthropogenic pollutant and, especially, aerosol emissions are highly non-homogeneous. The formation and transformation processes of aerosols with respect to concentration of particles and precursors and the gas-phase chemistry are highly non-linear; consequently, the scale at which the emissions, formation and transformation processes are resolved in models has a significant influence on the resulting concentration fields of the aerosols and gas-phase compounds.

Upscale cascade simulations can be performed using a combination of models resolving from the urban-mesoscale to the regional-global scale. The urban scale modelling is primarily intended to evaluate the source term and the role of the local processes in transformation of the primarily emitted aerosols. The mesoscale model can define intense sources like large cities and investigate the evolution of large urban plumes. These plumes are subgrid phenomena for the regional-global models that have the highest resolution (between 10 km and 100 km grid sizes) in the zoomed areas. Therefore, urban-mesoscale models can be applied to derive these subgrid parameterizations for the regional-global model. To understand the impact of aerosols and gas-phase compounds emitted from local/urban sources on the regional and global processes, three scales of the integrated atmosphere-chemistry-aerosol and general circulation models have to be considered: (i) local, (ii) regional, and (iii) global.

The elements of urban canopy (buildings, trees and transport) induce perturbations which affect on air quality. A detailed understanding of such perturbations is very important for the forecasting of pollutant dispersion. The substantial difference of geometrical and physical properties of the urban canopy elements leads to considerable variation of turbulent and mass fluxes. Therefore, microscale atmospheric models become important tool in air quality prediction in the last decade. To understand the physics of the transport phenomenon in an urban canopy, a large number of investigations have been carried out by means of field measurements (Yee and Biltoft, 2004), wind-tunnel experiment (Gerdes and Olivari, 1999; Kastner-Klein and Plate, 1999) and numerical simulations (Santiago et al., 2007; Nuterman et al., 2007). But only mathematical models allow the examination of flow patterns in detail, because it is difficult to describe all the variety of flow properties based on experiments or field observations. Nevertheless the air flow and pollutant dispersion data obtained from field and wind-tunnel experiments are usually important tools and provide the possibility of validating the numerical models (COST Action 732, http://www.mi.uni-hamburg.de/Home.484.0.html).

To show the complexity of urban air dynamics an investigation of aerodynamics of street canyons was performed basing on the GIS data (http://www.2gis.tomsk.ru). This geoinformation system contains the information on buildings arrangement/heights and motorways location in Tomsk, Russia.

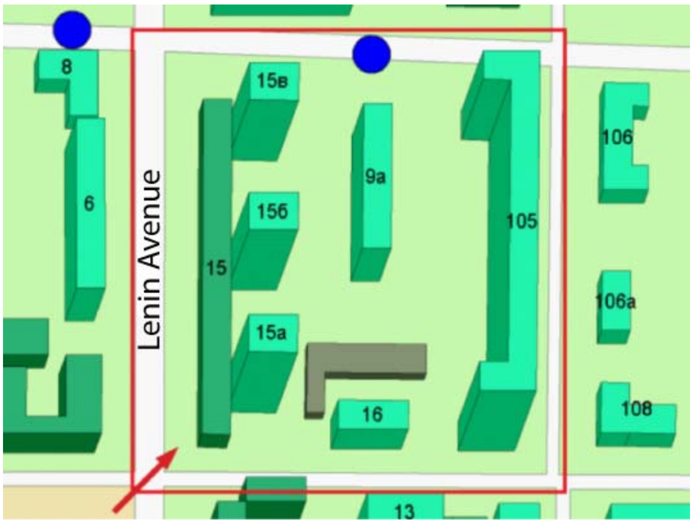


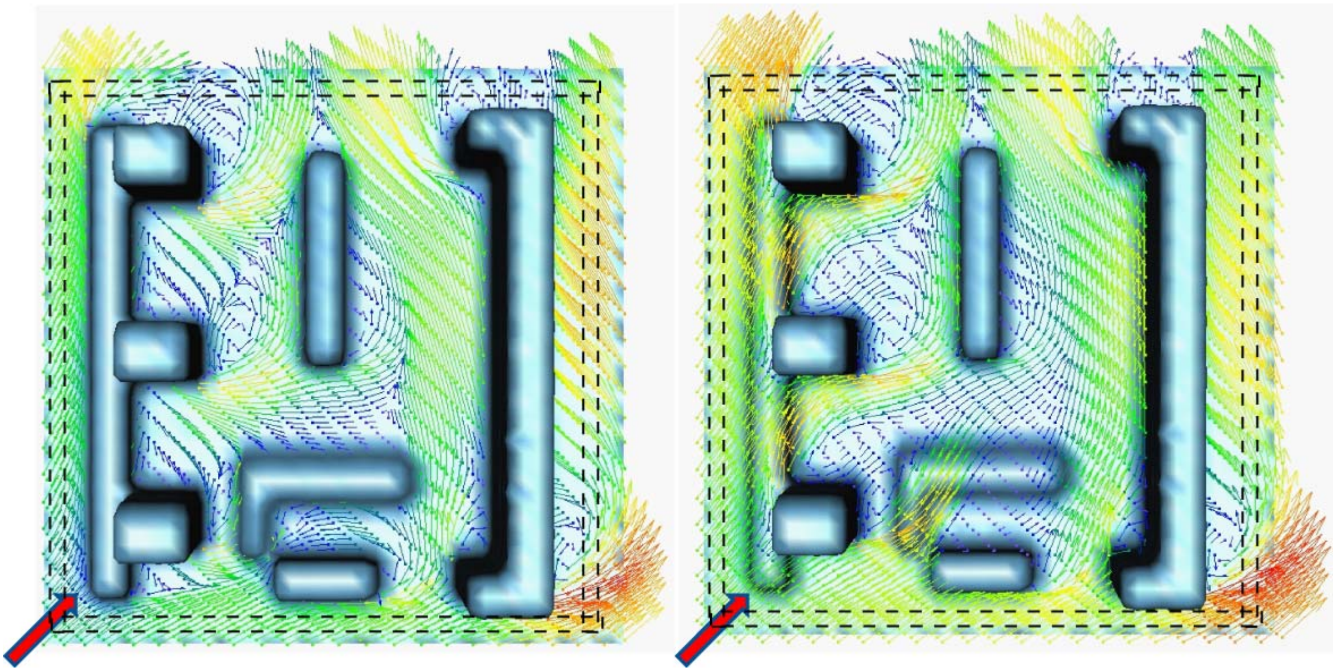
Figure 3.6.1. *Scheme of real urban area of Tomsk city: red rectangle is denoted the computational domain*

and the red arrow is wind direction

The computational domain is area with the length 260 m width 260 m and height 60 m. The inflow wind direction is south-west denoted by the red arrow (Figure 3.6.1). This direction was chosen due to the domination of the south-west winds in the summer time and the north-east in the winter time over Tomsk. The computational domain includes buildings with the different configurations and heights. The calculations were conducted on the non-uniform grid: 177 x 182 x 79 cells. The pollution sources (with constant intensity) are located along motorways. The inflow boundary conditions are:

$$U(z) = U_{ref}\left(\frac{z}{z_{ref}}\right)^{\alpha}, \; k(z) = \frac{u_*^2}{\sqrt{C_\mu}}, \; \varepsilon(z) = \frac{u_*^3}{\kappa(z + z_0)},$$

where α=0,16, u_*=0,38 m/s, z_0=0,05 m, U_{ref} = 5,5 m/s, z_{ref} = 9,0 m.



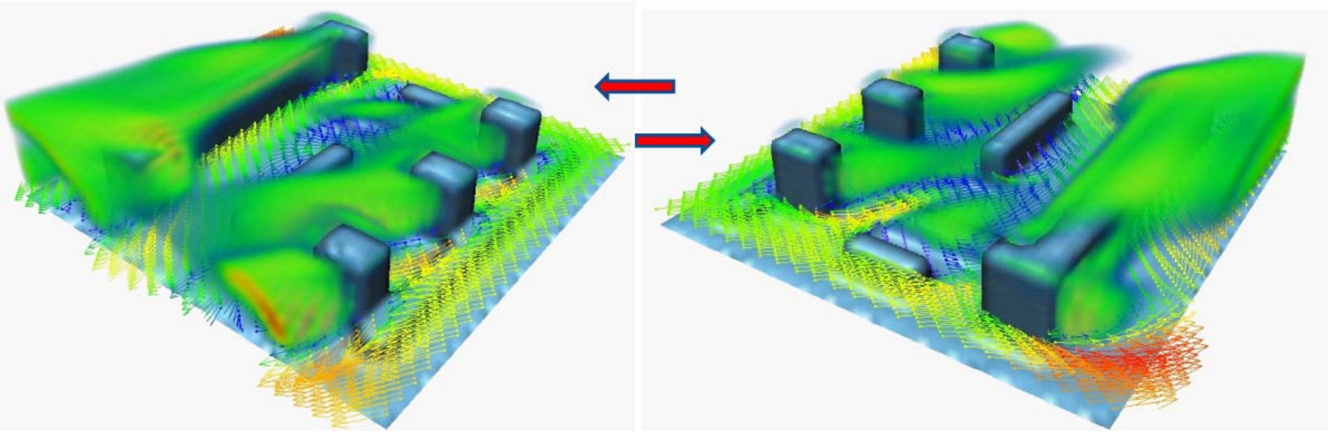
a) b)

Figure 3.6.2. *Vector field of velocity at z = 1,5 m (a) and at z = 7 m (b) for real urban area of Tomsk city (Nuterman, 2008); red arrows denote wind direction, dashed lines denote the location of roads/sources of pollution*

Vector fields, kinetic energy of turbulence and pollution concentration are presented on the figures 3.6.2-3.6.4. The results of computations show numerous vortexes in the corners and on the leeward sides of the buildings. The production of turbulent kinetic energy takes place at the frontal sides of the buildings and in the areas of rotational air motion (Figure 3.6.3). The calculations show that the turbulence level is usually higher at the roofs and the upper part of obstacles. The maximum of concentration is present along the roads but the increasing of local maximums is also observed in the secondary vortexes at near-ground level (Figure 3.6.4). It happens because the rotational air motion involves an impurity from the windward side and retains it on the leeward side. The pollution pattern is substantionally variated depending on the height.
One of the most important outcomes of microscale models for regional and global modelling is the vertical exchange between the urban canopy layer and the urban boundary layer. At now there are two possibilities of microscale models application for large scale modelling:

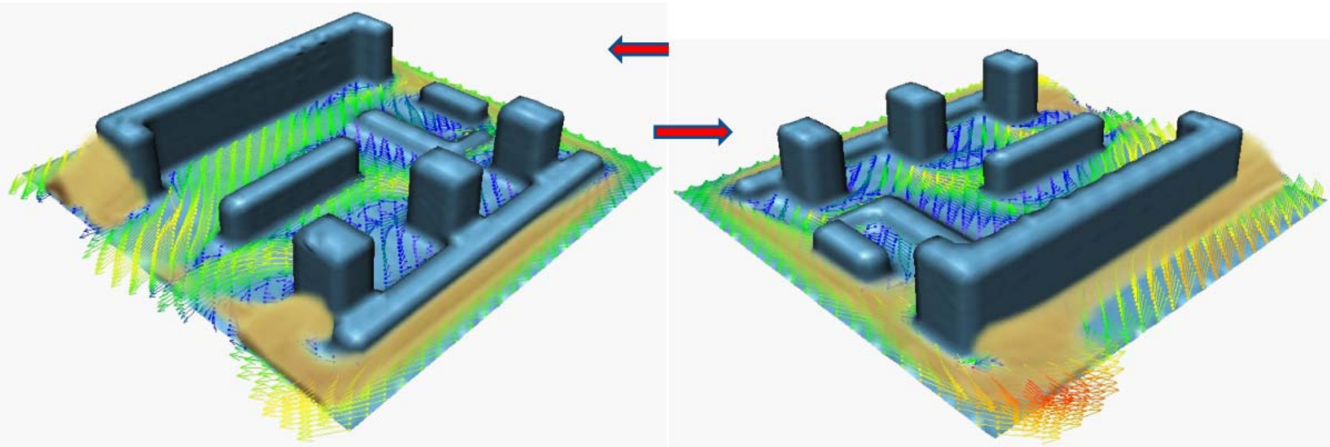
1. One way/two-way nesting – explicit resolving of urban canopy elements at sub-grid level of urban-mesoscale model.

2. Computation of drag coefficients and fluxes (Martilli, Santiago, 2007) for different types of urban obstacles and the addition of the forcing in the governing equations of urban-mesoscale models.



a) b)

Figure 3.6.3. *Volumetric visualization of kinetic energy of turbulence field for real urban area of Tomsk city (Nuterman, 2008); red arrows denote the wind direction*



a) b)

Figure 3.6.4. *Volumetric visualization of concentration field for real urban area of Tomsk city (Nuterman, 2008); red arrows denote the wind direction*

3.7. Source - receptor modelling for environment and health risk assessments

Estimation of regions with high potential risk/vulnerability from different risk sites is important for long-term planning socio-economical development of territories and emergency systems. The concept of ecological risk/vulnerability of territories with respect to anthropogenic impact is actively used in recent environmental investigations. The problem of risk assessment becomes especially urgent in connection with different accidents of radioactive, chemical and biological nature (e.g. due to terror acts). One of the most important aspects of this problem is the source term estimation for emergency response systems. E.g., after the Algeciras accident in Spain (30 May 1998) many European monitors measured peaks of radiation, but during several days the reason was unknown. A similar situation applies to the Chernobyl disaster.

Such accidents show the necessity to develop constructive methods for estimation of an unknown source term based on monitoring data, and prediction and assessment of risk/vulnerability levels for various risk sites and situations under conditions of both ordinary and extraordinary anthropogenic loads.

Methods of numerical modelling are widely spread for the solution of pollution problems, including the source-receptor relationship problem. Two approaches are usually used: Lagrangian and Eulerian. Lagrangian models allow calculating the trace of the individual particle or ensemble of particles moving together with air masses. Eulerian approach gives the distribution of concentration of pollutants, released from a given set of sources, in a chosen domain. These two approaches are not alternative; they supplement each other. Each approach has its own advantages and drawbacks and application areas.

Depending on the goal of investigation, forward and inverse procedures of modelling are distinguished. The methods of forward modelling are traditionally used for the solution of forecast and assessment problems. For their realization, the values of all input parameters of the models, boundary and initial conditions, sources of the external and internal forcing have to be given. Forward problems are used to study the processes of propagation of perturbations from various sources. These are so-called source-receptor problems. The spatial-time domains, where perturbations are observed, play role of zones-receptors.

The methodology of inverse modelling is mainly oriented towards diagnosis and solution of inverse problems. The Novosibirsk scientific school of Acad. G.I. Marchuk in Russia suggested a new, very elegant theoretical method for inverse modelling, based on variational principles with adjoint equations (Marchuk, 1982, 1995; Penenko, 1975,1981, Penenko and Aloyan, 1985) and suitable for both Eulerian and Lagrangian models (Penenko and Tsvetova, 1999).
Due to it, a special adjoint problem is formulated for the functional defined in the receptor-zone so that solving begins from the result (receptor) and moves to the sources and causes. From the viewpoint of ecological safety, the inverse problems of the receptor-source type are of interest, since they allow us to determine the degree of the potential danger of contamination of the zone-receptor by pollutants entering it and to identify sources of this danger. In combination with the forward modelling, the inverse approach opens up new prospects of extending the class of relevant problems and developing as well as organizing interactive technologies for their control and mitigation.

Source-receptor data can be evaluated: a) statistically or b) in combination with monitoring data to derive sources or other model variables. The common back-trajectory technique, suitable only for Lagrangian models, is an example of such inverse studies. Most of western scientists use these techniques for the discussed problem.

During the last decades, the methodology with adjoint equations becomes very popular among Western scientists as well (e.g., Robertson and Lange, 1998; Pudykiewicz, 1998; Baklanov, 2000).

In particular, the variational principles combined with decomposition, splitting and optimisation techniques are used for construction of numerical algorithms (Penenko, 1981; Baklanov, 1988). The novel aspects are the sensitivity theory and inverse modelling for environmental problems, which use the solution of the corresponding adjoint problems for the given set of functionals and models (Penenko, 1975, 1981, 1998; Penenko and Baklanov, 2001; Penenko et al., 2002). The methodology proposed provides optimal estimations for objective functionals, which are criteria of the atmospheric quality and (or) informative quality of measurements.

E.g., the Danish Emergency Response Model for Atmosphere (DERMA), developed by DMI originally in the direct mode, is also tested in the inverse (adjoint) mode for different resolutions and grid domains for forecast and for long-term simulation of source-receptor relationship for various pollutants including nuclear, chemical, biological etc. danger (Sørensen, 1998; Baklanov and Sørensen, 2001). Among 28 models from most of European countries, USA, Canada and Japan, which contributed to model validations based on the European Tracer EXperiment (ETEX), the DMI's DERMA model was emphasized as performing excellently (Graziani et al., 1998).

3.8. Complex environmental risk assessment and vulnerability evaluation

A new methodology for multidisciplinary probabilistic environmental risk and vulnerability assessments based on employing of the GIS technology was suggested in the Arctic Risk project (*AR-NARP, 2005; Baklanov et al., 2006a; Mahura et al., 2005; Rigina & Baklanov, 2002*) for estimation of nuclear risk to the population in the Nordic countries in a case of a severe accident at the nuclear risk sites (NRSs) (Fig. 3.8.1). The main focus was on the evaluation of the atmospheric transport and deposition of radioactive pollutants from NRSs with further integration of the trajectory and dispersion modelling results into the GIS environment for evaluation of risks/ consequences/ vulnerability/ etc. The methodology developed was based on a probabilistic point of view. The main question addressed was: *What is the probability for radionuclide atmospheric transport, deposition and impact to different neighboring regions and countries in case of an accident at a risk site?*

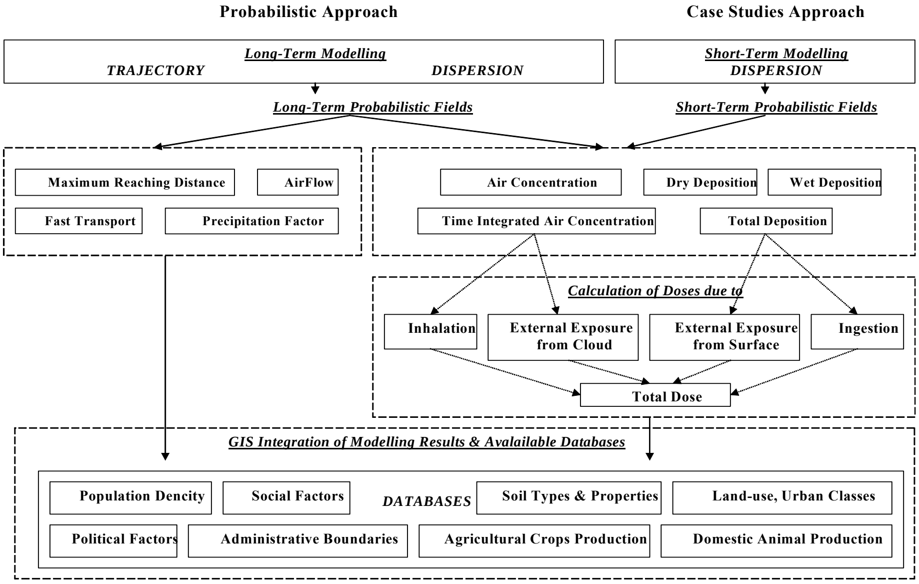


Figure 3.8.1. *General scheme of probabilistic assessment of the risk sites' impact.*

To answer this question a set of different approaches, methods, and research tools was tested and applied:

(i) *Trajectory Modelling* - to calculate multiyear forward trajectories originated over the locations of selected risk sites;

(ii) *Dispersion Modelling* - for long-term simulation and case studies of radionuclide transport from hypothetical accidental releases at sites;

(iii) *Cluster Analysis* - to identify atmospheric transport pathways from sites and its temporal variability;

(iv) *Probability Fields Analysis* - to construct annual, monthly, and seasonal risk sites impact indicators to identify the most impacted and sensitive geographical regions;

(v) *Specific Case Studies* - to estimate consequences for the environment and population after a hypothetical accident;

(vi) *Vulnerability Evaluation to Radioactive Deposition* - to describe its persistence in the ecosystems with a focus on the transfer of certain radionuclides into the food chains of key importance for the intake and exposure for a whole population and certain population groups;

(vii) *Risk Evaluation and Mapping* - to analyze environmental, social, economical, etc. consequences for different geographical areas and various population groups taking into account social-geophysical factors and probabilities, and using demographic and administrative databases based on GIS analysis.

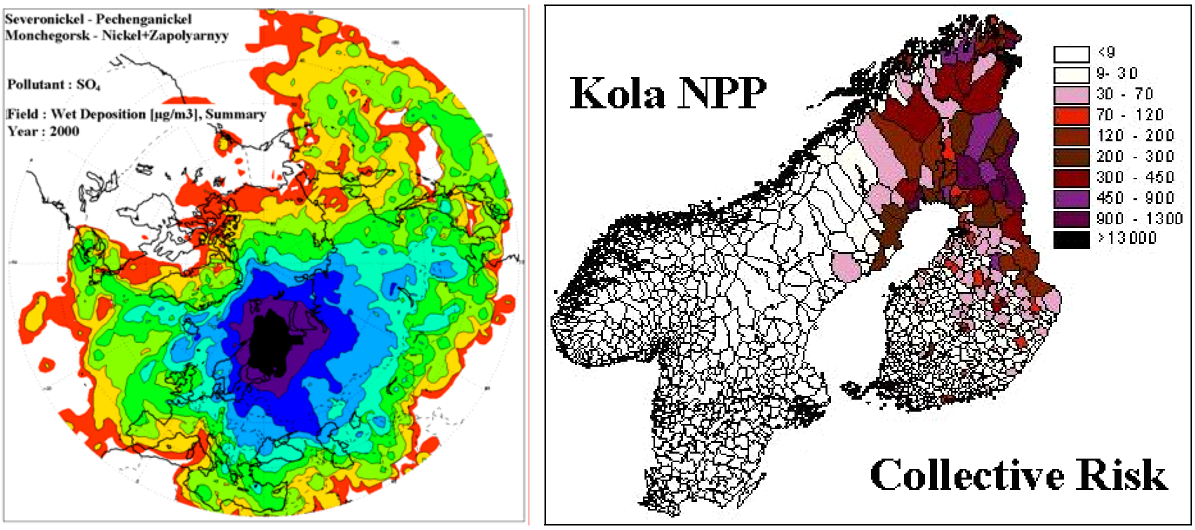


Figure 3.8.2. *(a) Annual summary wet deposition field for sulphates due to continuous anthropogenic emissions from three Cu-Ni smelters of the Kola Peninsula, Murmansk region, Russia; and (b) Collective risk for population in districts/provinces of the Nordic countries (Finland, Sweden, ad Norway) resulted from the hypothetical accidental release of Cs137 from the Kola nuclear power plant (NPP), Murmansk region, Russia.*

The developed methodology was tested on examples of the risk sites located in different geographical regions - Arctic, Sub-Arctic, Far East, and Northern Europe (see summary in *Baklanov et al., 2006b*). The sites included locations of the nuclear power plants' reactors (Mahura et al., 2005a), nuclear reprocessing plant (*Lauritzen et al., 2006; 2007*), nuclear submarine and decommissioning sites (*Mahura et al., 2005b; Yao et al., 2007*),and former nuclear weapons testing site (*Balakay , 2007*). Recently the methodology developments were extended to other types of environmental risk sites and mostly located in the Siberian and Ural regions of Russia, Kazakhstan, Uzbekistan and others (*Mahura et al., 2006*) and, in particular, for the chemical risk sites focusing on long-term as well as accidental emissions (*Mahura et al., 2007ab, 2008; Svetlov et al., 2007; Tridvornov, 2008*). An example of the long-term dispersion simulation employing the Danish Emergency Response Model for Atmosphere (DERMA) model, and the results of the risk calculation employing the GIS technology (ArcView) are shown in Fig. 3.8.2.

In particular, within the activities of this group "Atmospheric Pollution and Risks" of the Enviro-RISKS project, the DMI performed long-term simulation of atmospheric transport and deposition patterns from sources of continuous anthropogenic sulphates and radionuclides emissions located in the Siberian, Kazakhstan, Ural, and other geographical regions. One of the applications of this methodology and its integration into GIS risk-analysis is demonstrated on an example of the geoinformation modeling of radionuclide transfer from the territory of the Semipalatinsk Test Site in a separated Enviro-RISK report (*Zakarin et al., 2008*).

The DERMA was employed to perform simulations of air concentration, time integrated air concentration, dry and wet deposition patterns resulted from continuous emissions of chemical risk sites. The geographical locations of the Siberian chemical and metallurgical enterprises situated near the cities of Kemerovo, Norilsk, Novokuznetsk, Chelyabinsk, Ekaterinburg, Nizhniy Tagil, Kras-

noyarsk, Zheleznogorsk, and others were selected as representative sources of such emissions. To perform such simulations the European Center for Medium-Range Weather Forecasts (ECMWF) 3D meteorological fields (for years of 1985 - as climatologically typical year, and 1983 - as year with a significant deviation of atmospheric circulation patterns for the North Atlantic Oscillation) were used as input by the DERMA model. Several assumptions were applied. In particular, the hypothetical daily unit releases of sulphates at a constant rate were considered from each site. For each daily release the followed transport through the atmosphere and deposition on the underlying surface due to dry and wet removal processes were estimated on an interval of 2 weeks.
Detailed analyses of simulated concentration and deposition fields for each site allow evaluating spatial and temporal variability of these resulted patterns on regional and hemispheric scales (example is given in Figure 3.8.3). The results of these simulations are also applicable for GIS integration as well as essential input for further evaluation of doses, impacts, risks, short- and long-term consequences for population and environment from potential sources of continuous emissions.

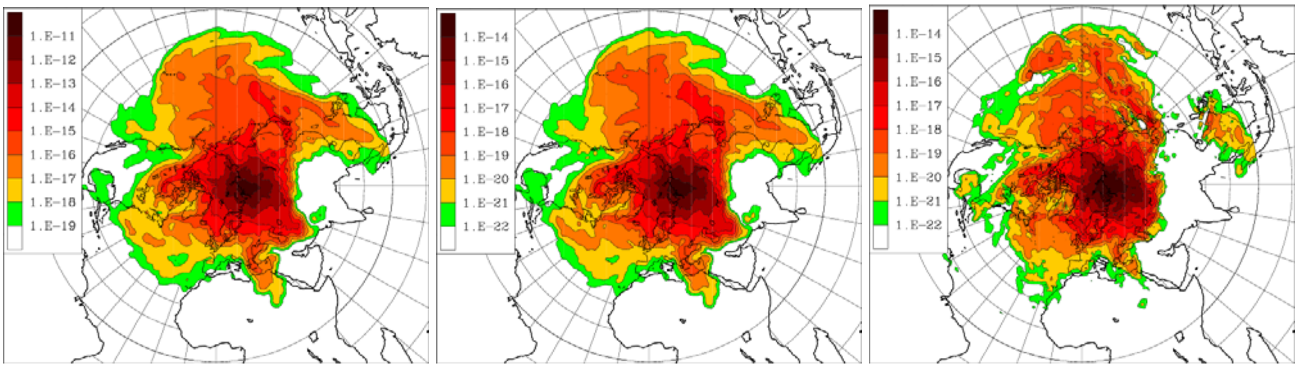


Figure 3.8.3. DERMA model results of the long-term dispersion modelling: annual time integrated air concentration, dry and wet deposition patterns from the Norilsk nickel plant.

3.9. Climate change and air quality modelling

Uncertainties in emission projections of gaseous pollutants and aerosols (especially secondary organic components) need to be addressed urgently to advance our understanding of climate forcing (Semazzi 2003). The role of greenhouse gases (such as water vapor, CO_2, O_3 and CH_4) and aerosols in climate change has been highlighted as a key area of future research (Watson et al 1997). In relation to aerosols, their diverse sources, complex physicochemical characteristics and large spatial gradients make their role in climate forcing particularly challenging to quantify. In addition to primary emissions, secondary particles, such as, nitrates, sulphates and organic compounds, also result from chemical reactions involving precursor gases such as SOx, DMS, NOx, volatile organic compounds and oxidizing agents including ozone. One consequence of the diverse nature of aerosols is that they exhibit negative (e.g. sulphates) as well as positive (e.g. black carbon) radiative forcing characteristics. Although much effort has been directed towards gaseous species, considerable uncertainties remain in size dependent aerosol compositional data, physical properties as well as processes controlling their transport and transformation, all of which affect the composition of the atmosphere. Probably one of the most important sources of uncertainty relates to the indirect effect of aerosols as they also contribute to multiphase and microphysical cloud processes, which are of considerable importance to the global radiative balance (Semazzi 2003).

In addition to better parameterization of key processes, improvements are required in regional and global scale modelling (IPCC 1996 and Semazzi 2003). Resolution of regional climate information from atmosphere-ocean general circulation models remains a limiting factor. Vertical profiles of temperature, for example, in climate and air quality models need to be better described. Such limitations hinder the prospect of reliably distinguishing between natural variability (e.g. due to natural forcing agents, solar irradiance and volcanic effects) and human induced changes caused by emissions of greenhouse gases and aerosols over multi-decadal time scales. Consequently, the current predictions of the impact of air pollutants on climate, air quality and ecosystems or of extreme events are unreliable (e.g. Watson et al 1997). Therefore it very important for future research to address all the key areas of uncertainties so as provide an improved modelling capability over regional and global scales and an improved integrated assessment methodology for formulating mitigation and adaptation strategies.

In this concern one of the important tasks is to develop a modelling instrument of coupled 'Atmospheric chemistry/Aerosol' and 'Atmospheric Dynamics/Climate' models for integrated studies (see Figure 3.9.1).

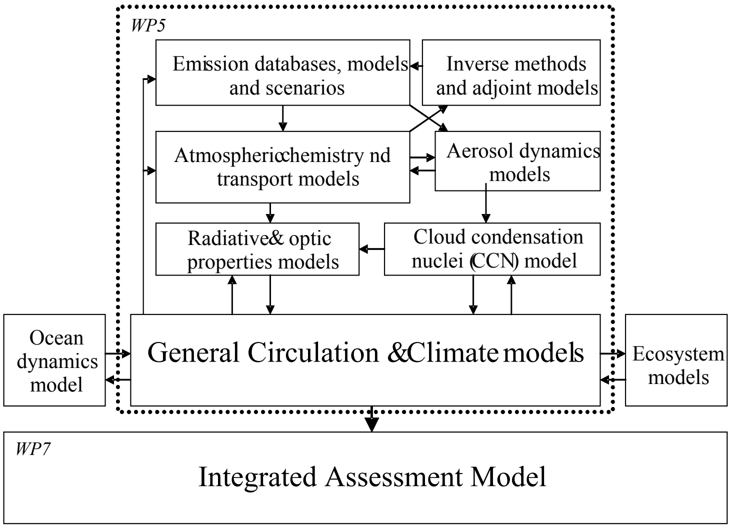


Figure 3.9.1. *The integrated modelling system structure for predicting climate change and atmospheric chemical composition.*

4. Interconnected Problems of Environment and Climate - Analysis of Dynamic Systems Evolution for the Goals of Prognosis and Design

Scenario approach is widely used in numerical modeling for the assessment of current and prospective states of environmental and ecological systems. The results of modeling essentially depend on the representation of the underlying hydrodynamics. We suggest a methodology for a quantitative description of the behavior of a dynamic system for a long time interval in a compressed, generalized form (Penenko and Tsvetova, 2008). Following it, the necessary information, intended to be used for the construction of scenarios, is extracted from a database containing measured and/or calculated data on hydrodynamic and environmental state functions.

4.1. State-of-the-art in the construction of informative basis systems

Analysis of environmental forecasting and projecting problems shows that they demand the assessment of possible nature changes for a long period of time. A way to solve such problems is the development of scenario approach. In this case it is natural to formulate environmental protection problems considering not only the direct impacts of the specific objects, but also the indirect effects arising additionally due to climate change. As a matter of fact, the goal of our work is formulated in the following way. A methodology should be created for incorporation of climatic data and some knowledge about assumed climate changes into environmental studies. To provide this, the climatic data should be presented in a compressed and generalized form. A deterministic "main" part extracted from the data under a given criterion of information completeness is implied here. To separate the scales of physical processes presented in the data, we propose a version of orthogonal decomposition method suited to the treatment of multidimensional, multivariate fields of data. The ideas of principal component analysis (PCA) and factor analysis (FA) are essentially used here.

The fundamental and applied aspects of PCA and FA are of interest for many researchers from the different areas of knowledge. The origins of the methods are related to the end of the 19th and the beginning of the 20th centuries. The different ways of PCA and FA are actively used in meteorology and oceanography from the middle of the last century. The systematic description of the main statements and some applications can be found, for instance, in the monographs of Harman (1976), Mescherskaya et al. (1970), and Preisendorfer (1988). The voluminous bibliography containing more than a thousand of papers with surveys of the history, theoretical background and practical applications are presented there, too.

The limiting parameter for these methods is the dimension of the data analyzed. In practice, these algorithms are very sensitive to the increase of the dimensions of eigenvector problems (EVP). Some existing approaches reducing the dimensions are discussed in details by Mescherskaya et al (1970) and Preisendorfer (1988). Among different algorithms, the eigenvector-partition methods should be mentioned. In such algorithms, the data are divided by parts and the total EVP is replaced by several EVPs of low dimensions. Then the solution is obtained by constructing the basis from the separate parts.

The problem of the informative bases construction holds a priority for many years. Lorenz (1965) used singular vectors of the linearized operator of a simple model to study the flow-dependent predictability. An application of bi-orthogonal decomposition method to the meteorological fields with the use of EVP of the linearized forward and adjoint operators of atmospheric hydrodynamics was considered by Marchuk (1968). Recently the other approaches for optimal representation of the perturbations have been intensively developed for the ensemble weather prediction. The singular vectors of the tangent linear operators associated with forecasting models were used by Molteni and Palmer (1992), Mureau et al. (1992), Ehrendorfer and Tribbia (1997), Gelaro et al. (1998), Kim et al (2004). Toth and Kalnay (1997) applied the bred vectors for generation of perturbations. For quantitative estimations of a model sensitivity degree to initial data and for construction of scenario ensembles, the Lyapunov exponents and vectors are used as well. This approach possesses an advantage that it is applied to the non-linear models.

Some methods of orthogonal and bi-orthogonal bases construction for implementation of variational principles in the problems of atmospheric dynamics can be found in (Penenko, 1974; 1975; 1981).

Here we present a methodology of orthogonal decomposition for analysis of the large databases which describe the behavior of the multidimensional dynamic systems both linear and non-linear ones. The kernel element of the methodology is the solution of EVP. It should be noted that our methodology differs from the above mentioned eigenvector-partition methods (Preisendorfer, 1988; Mescsherskaya et al., 1970). We organize the data in such a way to avoid splitting the EVP and to solve the problem of searching for the main components without loss of information quality. A distinctive element of our approach is a two-level structuring of the analyzed database. This allows us to solve the decomposition problem practically without limitations on amount of data.

Quantitative information of atmospheric and ocean circulation for long time periods can be found in the high capacity databases such as reanalysis. For example, information on the basic state variables of the climatic system and some other characteristics are collected in the NCEP/NCAR reanalysis database (Kalnay et al., 1996). In this study, we have considered this database as the description of the concrete realization of the climatic system evolution. And a data subset for 56 years has been used here as the climatic background. In the presented example on decomposition of the reanalysis database, a two-level structuring with respect to time scales has been made. This gives the possibility of producing the time-dependent dynamical bases that is convenient for prognostic goals. In frames of our approach, the other variants of structuring are also possible. To realize the methodology, an efficient computational technology has been developed to be used for climate studies and for organizing the scenarios for environment protection and design.

4.2. Functionals and variational principles for analysis of the phase spaces

To solve the above mentioned problems, we need to formulate some goal functionals for short description of the generalized characteristics of the state variables of complicated dynamic systems. The form of such functionals is conveniently chosen from the statements of mathematical models of the processes under discussion. Without going into details, we use a model in which dynamics of the atmosphere as well as transport and transformation of impurities are presented. The structure of such a model can be given in the operator form (2.1).
The problems of environment quality diagnosis and forecasting are of multi-goal character. Therefore, such methodology of modeling is necessary which can be adapted to the divers statements and criteria. To provide this, a set of generalized characteristics is introduced into the model system. The characteristics for quantitative estimations are given as the functionals (2.8) .
The required estimates of the functionals and their variations are obtained with the help of the adjoint sensitivity relations for the chosen set of functionals (2.8). The spatial and temporal dynamics of these relations in $Q(D_t)$ and $R(D_t)$ is expressed by means of the sensitivity functions (SF) of analyzed functionals with respect to variations of the model parameters. To jointly analyze data, models, and SFs, the agreed definitions of "energy" inner products in corresponding functional spaces have to be used.
For instance, if the quasi-static model of hydrodynamics is taken, the energy inner product for the state functions can be chosen in the form

$$(\varphi,\varphi^*)_{Q(D_t)} = \int_{D_t} \left\{ uu^* + vv^* + \sigma_0 \left[TT^* + (\gamma(p)/R^2)HH^* \right] \right\} dDdt + \sum_{i=1}^{n_f} \int_{D_t} \beta_i \varphi_i \varphi_i^* dDdt, \quad \mathbf{(4.1)}$$

where $\varphi = \left(u, v, T, H, \left(\varphi_i,\ i = \overline{1, n_f}\right)\right)$ is the vector-function of the state variables, u, v are the horizontal components of the velocity vector, T is temperature, H is geopotential height, φ_i are the components of hydrological cycle, admixtures in the gaseous state, and aerosols, n_f is the total number of substances, R is the universal gas constant, and σ_0, $\gamma(p)$, β_i are weight factors. The detailed description of the variational form of models by means of the integral identity can be found in (Penenko, 1981; Penenko and Tsvetova, 1999).
To study sensitivity functions, let us introduce an inner product agreed with (2.8),(4.1) and generated by the right side of the sensitivity relations (2.14) for the functionals $\Phi_k(\varphi)$ (Penenko, 1981). For convenience we present it in the form:

$$\delta\Phi_k^h(\varphi) \equiv (\mathrm{grad}_{\mathbf{Y}}\Phi_k^h(\varphi), \delta\mathbf{Y}) \equiv \frac{\partial}{\partial\alpha} I^h(\varphi, \mathbf{Y} + \alpha\delta\mathbf{Y},\ \varphi_k^*)\big|_{\alpha=0}\,; \quad \mathbf{(4.2)}$$

$$\delta\mathbf{Y} = \eta\, \mathrm{grad}_{\mathbf{Y}}\, \Phi_k^h(\varphi), \quad k = \overline{1, Kc}\,. \quad \mathbf{(4.3)}$$

Here a, h are real parameters; $\delta\mathbf{Y}$ are variations of the model parameter vector that are chosen to be proportional to SFs; φ is the solution to the direct problem (1) with prescribed values of the set of parameters $\mathbf{Y}$; φ_k^* are solutions to the adjoint problems generated by variational principles to estimate the variations of the augmented functionals $\tilde{\Phi}_k^h(\varphi)$ (2.12), (2.,13). The derivative in (4.2) is considered in Gateaux sense (Lévy, 1951). The initial data and uncertainty functions are included into the number of components of the parameter vector $\mathbf{Y}$. The structure of the phase space of SFs defined by the right side of (4.3), is determined by the structure and dimensions of the components of parameter vector and by the form of integral identity functional which is the variational form of the processes model (2.5).

Thus the functionals of four main types participate in the variational principle. They are defined as the inner products (2.5),(2.8),(4.1), (4.2). For the aims of orthogonal decomposition, the functionals of energy type (4.1) and (4.2) are directly used. The first of them defines the metrics and norm in the space of state variables. The second one introduces the metrics and norm in the phase spaces of SFs.

4.3. Methodology of database analysis

To analyze a high dimension database describing the evolution of the processes examined, we apply the methods of orthogonal decomposition. The starting point to this aim is the definition of the database structure. The form of the total energy inner product is taken into account. This gives the metrics and type of the functionals in the space of analyzed fields which, in terms of (4.1),(4.2), are multidimensional and many-component aggregates of high dimension. The meteorological fields can be the results of observations of the nature processes, as well as the results of model runs. Although the model might be nonlinear with respect to the state functions and parameters, we assume that the calculated fields belong to the linear vector spaces. Such approach is due to the fact that the quantitative description of the non-linear behavior of the dynamic systems can be given in the form of multidimensional linear vector space.

4.4. Database structuring

So, let these fields be the vector-matrix objects in the real linear spaces. The set of vectors is defined as

$$\left\{\varphi(\mathbf{x},t,\mathbf{Y}) \in Q(D_t);\left(\mathbf{x},t\right)\in D_t;\mathbf{Y}\left(\mathbf{x},t\right) \in R(D_t)\right\}. \tag{4.4}$$

For organizing the algorithms, we arrange the database in the form of a block matrix. To describe the blocks, two groups of independent variables-indices are introduced. The first group describes the governing (external) structure of the data: the number of blocks and their order in the overall hierarchy. The second group defines the numeration and location of the components inside each block. Thus, the vectors can be presented in the block form as

$$\varphi = \left\{ \varphi_i(k) \right\},\ \varphi_i(k) \in R_N,\ i = \overline{1,n},\ n \geq 1,\ k \in K, \tag{4.5}$$

where n is the number of blocks in the external structure; K is the set of values of the multi-indices k of the components in the internal structure of each block. The total number of elements in the internal structure is denoted by N. Hereinafter, all operations are performed in the real vector spaces R_N and R_n with corresponding inner products.

It should be noted that all algorithms are universal, and the specific features of each problem are determined by the structure of the data matrix and by the form of the inner products.
Let the energy inner product be:

$$\left(\varphi_i,\varphi_j\right) = \left\langle \varphi_i(k), C\varphi_j(k)\right\rangle = \left\langle C^{1/2}\varphi_i(k), C^{1/2}\varphi_j(k)\right\rangle,\ i,j = \overline{1,n},\ k \in K. \tag{4.6}$$

Here C is the diagonal $N \times N$-matrix whose elements contain the scaling factors and the volume metrics in the discrete representation of the functionals (5)-(7). It should be stressed that the calculation of inner product is the key element which is responsible for the accuracy of solution to the decomposition problem.

Now we introduce the transformation of the state variables of the form $\mathbf{Z}_i = C^{1/2}\varphi_i$ so that the components of vectors in the new form should have the identical physical dimension and energy property. The dimensions of the inner product (10) and norms should remain unchanged. Finally, the database for solving the problem can be presented as $(n \times N)$-matrix $Z = [\mathbf{Z}_i],\ i = \overline{1,n}$, where n is the number of vector columns. Each column contains the complete internal structure with total number of components being equal to N. The quantities n, N, and the content of the set of multi-indices K are the input parameters for structuring the database Z and forming the inner product (10). The obtained vectors are centered with respect to a given center vector which is introduced as input parameter of the algorithm. In particular, the vector of the sampling mean can be used as the center. Then the vectors are reduced to the unit length in the norm defined by the inner product.

The data matrix Z can be considered in two ways: as the set of n vector-columns $\{\mathbf{Z}_i,\ i = \overline{1,n}\}$ from R_N, and as the set of N vector-rows $\{\mathbf{V}_q,\ q = \overline{1,N}\}$ from R_n. Hence, we can use two Gram matrices: the $(n \times n)$ - matrix $\Gamma = Z^{\mathrm{T}}Z = \{\Gamma_{ij} = (\mathbf{Z}_i, \mathbf{Z}_j),\ i,j,= \overline{1,n}\}$ and the $(N \times N)$ -matrix $M = ZZ^T = \{M_{ij} = (\mathbf{V}_i, \mathbf{V}_j),\ i,j,= \overline{1,N}\}$ (the superscript T indicates transposition). The Gram matrices are real, symmetric and positive semi-definite. It is known that $r \equiv \mathrm{rank}(\Gamma) = \mathrm{rank}\ (M) \le \min(n,N)$. To make the algorithm efficient, we organize the source database so that n should be much less than N. And all the calculations are made with the $(n \times n)$ - matrix Γ. In this case, the value of the parameter n can be limited only by the capabilities of the procedures used for solving the EVP for the matrix Γ. The size N of the vectors belonging to the internal structure can be as large as desired.

4.5. Quadratic forms and decomposition with respect to the scales of disturbances

Construction of multidimensional orthogonal spaces is a fundamental problem of functional analysis and linear algebra. In addition to Gram matrices, the effective tools for studying the linear transformations of vector fields and the corresponding databases are bilinear and quadratic forms (Courant and Hilbert, 1953, Gantmacher, 1959). Let us introduce the quadratic form joining the matrices Z and Γ:

$$S(\mathbf{V}, Z) \equiv (Z\mathbf{V})^T (Z\mathbf{V}) = \mathbf{V}^T Z^T Z\mathbf{V} = \mathbf{V}^T \Gamma \mathbf{V}. \qquad (4.7)$$

This form is defined on the space of vectors $\mathbf{V} \in R_n$, which satisfy the condition $\mathbf{V}^T\mathbf{V} = 1$. In essence, the quadratic form characterizes the scattering of the sample with respect to the given center vector (Wilks, 1962). The Gram matrix Γ is also referred to as scatter matrix.

Then using the methods for studying the extreme properties of the form $S(\mathbf{V}, Z)$, we perform the orthogonal decomposition of the space of vectors forming the matrix Z and belonging to $R_N \times R_n$. Omitting the description of intermediate stages, we obtain the solution to the problem as a set of orthogonal subspaces

$$\left\{ \begin{matrix} \mathbf{\Gamma v} = \lambda \mathbf{v}, \quad \lambda_p, \mathbf{v}_p \in R_n, \quad \mathbf{\Psi}_p(k) = \lambda_p^{-1} \sum_{j=1}^{n} v_p(j) \mathbf{Z}_j(k), \\ \mathbf{v}_p^{\mathrm{T}} \mathbf{v}_q = \lambda_p \delta_{pq},\ \mathbf{\Psi}_p \in R_N, \quad \mathbf{\Psi}_p^{\mathrm{T}} \mathbf{\Psi}_q = \delta_{pq},\ p,q = \overline{1,n} \end{matrix} \right\}. \qquad (4.8)$$

Here $\lambda_p \ge 0$; $\mathbf{v}_p$ are the eigenvalues and eigenvectors of the $(n \times n)$ Gram matrix Γ; δ_{pq} is Kronecker delta function; $\mathbf{\Psi}_p$ are the orthogonal basis vectors-subspaces (OBV) obtained by projection of the vector-rows $\{\mathbf{V}_i,\ i = \overline{1,N}\}$ of the matrix Z onto the basis of principal components

(PC) $\left\{\mathbf{v}_p, p=\overline{1,n}\right\}$. The internal structure of the vectors $\mathbf{\Psi}_p$ is the same as that of the vector-columns $\left\{\mathbf{Z}_i, i=\overline{1,n}\right\}$ of the matrix Z in the space R_N.

The value of λ_p can be taken as an information measure of the pair $\left\{\mathbf{v}_p, \mathbf{\Psi}_p\right\}$. An information index of the pair is defined as $\mu_p = (\lambda_p / \sum_{i=1}^{n} \lambda_i)$. The smallest eigenvalue $\lambda_n \geq 0$ is usually referred to as the measure of linear independence of the vector system (4.4). It does not grow if the number of vectors n in the system increases. The largest eigenvalue λ_1 characterizing the maximum scale of perturbations, does not decrease with the increase of n. Detailed studies of the vector systems and the corresponding Gram matrices can be found in (Taldykin, 1982).
The basic algorithms are given in (Penenko and Tsvetova , 2008).

4.6. Energy criteria for revealing the areas of the prescribed level of significance

The criteria are useful for revealing the regions of increased risk and vulnerability, as well as for detection of the centers of energy activity in the climatic system and risk/vulnerability zones. Following the definitions from (Buizza and Montani, 1999), let us denote the energy of the vector $\mathbf{\Psi}$ in the sub-domain identified by the multi-index $k \in K$ in (4.5) as $\gamma^c(\mathbf{\Psi}, k) = \left[\mathbf{\Psi}, \mathbf{\Psi}\right]_k$ and define

$$A \equiv \gamma^c(\mathbf{\Psi}, k_0) = \max_{k \in K} \gamma^c(\mathbf{\Psi}, k). \tag{4.9}$$

Here $\mathbf{\Psi}$ is one of the vectors from (4.4), (4.5), (4.8) or from their linear combinations and k_0 is the multi-index of localization of the maximum value of the function. Using these definitions, the region in which

$$\gamma^c(\mathbf{\Psi}, k) \geq \alpha A, \; k \in K_0^\alpha(\mathbf{\Psi}) \subset K \tag{4.10}$$

is calculated. Here α, $(0 < \alpha < 1)$ is a parameter chosen for extracting the region having the given relative level of energy significance. If the inner product (4.1) is chosen, the analysis of the region pattern $K_0^\alpha(\mathbf{\Psi})$ in dependence on the parameter α is used for assessment of the energy active regions. If the inner product (4.2)-(4.3) is taken, the regions of increased sensitivity/risk/vulnerability in the global climatic system or in its parts can be revealed .

4.7. Information content and physical meaning of orthogonal basis spaces

The decomposition algorithms and their results are used in various practical applications. The specific interpretation of the triplets $\left\{\lambda_q, \mathbf{v}_q, \mathbf{\Psi}_q,\; q=\overline{1,n}\right\}$ obtained from the system of orthogonal decomposition (4.4) depends on many factors such as: the goal of the study, the content of the database, the way of data structuring, and the concrete form of the energy inner product. Following the terms accepted in PCA and FA (Harman, 1976; Preisendorfer, 1988), the set of the eigenvectors $\mathbf{v}_q \in R_n$ can be conditionally related to the PCs, while the OBVs, $\mathbf{\Psi}_q \in R_N$, can be considered as the main factors which are a generalized version of the empirical orthogonal functions (EOFs) for multidimensional and multicomponent spaces of the complicated inner structure which is introduced by the given energy inner product.

The trace of Gram matrix is equal to the value of the total variance σ^2 of the source set Z. Owing to normalization of the vector-deviations to the unit length, we have: $\Gamma_{qq} = 1$, and $\mathbf{tr}(\Gamma) = n$. The part of the total variance equal to 1 falls on each vector block $\mathbf{Z}_i(\mathbf{x},t)$ of the initial set.

The physical dimensions of the elements of Γ coincide with those of the eigenvalues λ_q. They are defined by the dimension of "energy" which we imply in the functionals of the inner product. The dimensions of the components of the eigenvectors $\mathbf{v}_q$ follow the relation (4.8) and are equal to those of the square root of energy or, in terms of standard deviation, $\sigma_q = \sqrt{\lambda_q}$.

The value of λ_q is equal to the fraction of the total variance relating to the vector $\mathbf{v}_q$. As $\sum_{\beta=1}^{n} v_q^2(\beta) = \lambda_q$ from (4.8), each component $v_q(\beta)$ is equal to the standard deviation that defines the fraction of the input of $\mathbf{Z}_\beta(\mathbf{x},t)$ into the OBVs $\mathbf{\Psi}_q(\mathbf{x},t)$.

The components $v_q(\beta)$ of the vector $\mathbf{v}_q$ define the values of the projections of each vector-column of the matrix onto the OBV-basis. In other words, the vectors $\mathbf{v}_q$ characterize the variability of the initial sampling with respect to the constructed OBV-system. Owing to norm in (4.8), the basis functions $\mathbf{\Psi}_q(\mathbf{x},t)$ are dimensionless. They describe the time-space distribution of the total variance λ_q in fractions of the standard deviation σ_q over the region D_t^h and, hence, they characterize the relative measure of variability of the processes at each point of the grid domain.

4.8. Principles of prognostic scenarios organization for environmental studies

We propose that the climatic information should be taken into account for environmental forecasting by means of the special scenarios. In them, the results of orthogonal decomposition are involved for calculation of the hydrodynamic background along which the processes of transport and transformation of substances flow. The analysis of the main factors in the global and regional scales fulfilled jointly with the sensitivity analysis of the environment quality functionals, shows that the adequate simulation of the regional processes is impossible without their interconnection with global processes. For instance, this fact becomes strictly apparent while assessing the areas of ecological risk/ vulnerability for the protected region with respect to harmful impact (Penenko and Tsvetova, 2005, 2007a,b). Hence, the modeling technology is organized on the principles of combining the different scales models and of decomposing the state function on the background and perturbations. The essence of the technology is as follows. New elements named the guiding phase spaces are introduced into the model. These are the multicomponent fields of the space-time structure. They provide the description of the background structure with desired degree of information completeness with respect to the global climatic system state. The composition of the components depends on the form and the content of the state function of the model. These fields are used in the technology by means of the assimilation procedures. The current state, generated by the model, is calculated with allowance for the background processes prescribed by the leading spaces.

4.9. Deterministic and deterministic-stochastic (probabilistic) scenarios

As stated above, for construction of the guiding phase spaces which participate in the formation of the hydrodynamics background, the method of orthogonal decomposition is used. Let us define the guiding spaces as the sum of two constructive elements:

$$\boldsymbol{\varphi}_d(\mathbf{x},t) = \boldsymbol{\varphi}_d^0(\mathbf{x},t) + \boldsymbol{\varphi}_d^1(\mathbf{x},t), \ (\mathbf{x},t) \in D_t^{hd}. \tag{4.11}$$

Here $\varphi_d^0(\mathbf{x},t)$ is a large-scale part expressed by the linear combination of the leading basis subspaces in frames of orthogonal decomposition (4.8); $\varphi_d^1(\mathbf{x},t)$ is the space built on the components of the smaller scales; D_t^{hd} is the given set of points in D_t. The constituent $\varphi_d^1(\mathbf{x},t)$ may be deterministic- stochastic in the range of variability of the corresponding parameters from the database. For calculation of the stochastic part one may apply the probabilistic density functions of the state vectors defined in the phase spaces spanned by the leading set of the PCs and OBVs.

The use of the orthogonal decomposition results allows the scenarios for the typical and extreme situations to be formed. The quantitative measure of the basis information significance gives the possibility to classify the processes with respect to the scales of perturbations as well as to identify the spatial-temporal domains of perturbations with respect to the intensity of their development.

Forming the leading phase space with allowance for observation data on the sub-domain.

Let a set of the measured values $\mathbf{Z}^m(\mathbf{x},\tau)$ of the state vector be given in a sub-domain $D_\tau^m \subset D_t$. Then for approximate reconstruction of the vector $\mathbf{Z}$ in D_t, we use the algorithm

$$\mathbf{Z}(\mathbf{x},t)=\sum_{p=1}^{n_a} a_p^m \boldsymbol{\Psi}_p(\mathbf{x},t),\quad (\mathbf{x},t)\in D_t,\quad n_a \le n. \tag{4.12}$$

The coefficients of expansion $\mathbf{a}=\left\{a_p^m,\ p=\overline{1,n_a}\right\}$ can be found from the condition

$$\min_{\langle \mathbf{a}_p^m \rangle}\left\| \mathbf{Z}^m(\mathbf{x},\tau)-\sum_{p=1}^{n_a} a_p^m \boldsymbol{\Psi}_p(\mathbf{x},\tau)\right\|_{D_\tau^m}^2,\quad (\mathbf{x},\tau)\in D_\tau^m,\quad n_a \le n. \tag{4.13}$$

Here $\|\cdot\|_{D_\tau^m}$ denotes the Euclidean norm of vectors, given on D_τ^m, with a positive diagonal weight matrix W^m. Finally, the coefficients are obtained as

$$\mathbf{a}=\left(\Gamma^m\right)^{-1}\mathbf{F}^m,$$

$$\Gamma^m=\left\{\Gamma_{pq}^m=\left(\boldsymbol{\Psi}_p, W^m\boldsymbol{\Psi}_q\right)_{D_\tau^m},\ p,q=\overline{1,n_a}\right\},\quad \mathbf{F}^m=\sum_{p=1}^{n_a}\left(\boldsymbol{\Psi}_p, W^m\mathbf{Z}^m\right)_{D_\tau^m}.$$

Here $(\cdot,\cdot)_{D_\tau^m}$ is the inner product of vectors defined on D_τ^m with the weight W^m. It introduces the norm for (4.13), and Γ^m is a positively definite symmetric $n_a \times n_a$ Gram matrix for the system of vectors obtained by projection or interpolation of the values of basis vectors $\boldsymbol{\Psi}_p$ onto the set D_τ^m.

If the time interval τ is less than the interval t, on which the basis $\boldsymbol{\Psi}_p$ is defined, then the relation (4.12) has the prognostic character for calculation of the state variables by means of the basis in D_t.

The problem of reconstruction of meteorological fields with missing data are typical everywhere and especially in Siberia where the monitoring net is rare and non-regular in space. The advantage of using the informative bases for reconstruction of the system state by means of the observed data should be stressed. In this case, to solve the problem, we need only the number of observations which is commensurable with the number of the basis functions. This amount of data is enough for estimation of the expansion coefficients of the sought fields onto the informative basis. The combination of this approach and data assimilation procedures gives effective low-cost computational algorithms. Note that the availability of reconstruction of the field structure on insufficient data by means of data assimilation was firstly demonstrated at the Joint IUTAM/IUGG International Symposium on Monsoon Dynamics, New Dheli, 5-9 December, 1977 (Marchuk and Penenko, 1981).

4.10. Analysis of the scenario ensembles

In this section, some possibilities of application of the proposed methodology for the analysis of scenarios results are discussed. It is implied that the results are collected in a database in an unified form.

Let us consider a set of scenarios simultaneously and jointly. For this purpose we define a functional space of the scenarios results (FSS) and an energy inner product on it. Then we form the matrix Z , the scattering function $S(\mathbf{V}, Z)$, and the Gram matrix Γ . The ordinal numbers of scenarios are identified with the numbers of vector-columns in the matrix Z . These numbers is used as the variable of external structure. The content of the column is the result of the corresponding scenario.

Further all operations are produced in accordance with the general scheme of decomposition algorithm.

While calculating vectors $\mathbf{\Psi}_p$, the PCs show the relative input of each scenario in the formation of the OBV's basis. In its turn, the fraction of each OBV is reflected in the result of each scenario. The pairs (PCs, OBVs) present the general characteristics of the ensemble ranged by the degree of significance quantified by the eigenvalues of the Gram matrix.

The proposed scheme of collective analysis of the scenarios can be applied to the generalized studies of the quality of different models which are developing for the solution of the same class of problems. The interesting point might be the assessment of the generality of the different model results. It should be noted that the appropriate metrics has to be chosen. As a result, the PCs give a quantitative estimate of the relative role of each model in the formation of the general description of the processes under study. Moreover, they show how the constructed set of the OBVs is reproduced in the results of each model. The potential applicability areas of such analysis could be the ensemble weather prediction projects and the climatic projects, like the Atmospheric Model Intercomparison Project (AMIP) (Philips, 1994) and the Coupled Model Intercomparison Project, (CMIP) (Mehl et al., 2000).

5. Some Applied Environmental Problems

5.1. Studies of climate variability for revealing the areas of increased environmental risks

The problems of the long-term environmental forecasting demand to reveal the dynamical active zones and the areas of increased sensitivity to the variations of parameters (forcings). The methodology described above is suitable for studying such kind of problems. Here we demonstrate the implementation of the methodology to analyze the long-term behavior of the global climatic system. Decomposition with respect to the scales of processes allows one to identify activity centers and to use this information to formulate the problems of risk/vulnerability for sources/receptors keeping in mind their connection in the frames of (4.2)-(4.3). Some illustration are given in (Penenko, 2003, Penenko and Tsvetova,2007) and in item 5.4. To this end we use the NCEP/NCAR reanalysis database (Kalnay et al., 1996) which is a well-structured universal-purpose information system containing the basic set of atmospheric characteristics. This database is actively used for different goals. As for orthogonal decomposition, for instance, the monthly mean EOFs have been recently computed for studies of multiple regimes and low-frequency oscillations in the Northern Hemisphere's zonal-mean flow (Kravtsov et.al, 2006).
In our study the data for the period from 1950 to 2005 (56 years) are considered. The chosen time

interval is greater than the period of 30 years normally used in climatic estimates (IPCC, 2001). By example of these data, we make the problem formulation more definite and identify the main elements of the technique used.

To organize the study and to ensure efficient operation of the algorithms, we form a database as a subset of the reanalysis database and define the matrix Z and the quadratic form (4.7) in a suitable manner. The physical content of the components is selected in accordance with the goal functionals (2.8), inner products (4.1)-(4.2), and functionals (4.6) for calculation of the Gram matrix elements. Having in mind the accepted two-level structuring (4.4)-(4.6), we introduce two scales in time: external and internal. The external scale has the total duration of 56 years ($n = 56$) with time step of one year. As for internal scale, there are many variants beginning with a few days to a year. From the formal point of view the annual interval is the simplest one. But the loss of information quality may arise in the calculation of inner products (4.6) due to summing the huge number of data. Taking this fact into account and realizing our wishing to study the seasonal behavior of the climatic system, we choose a variant in which the annual interval is divided into 12 parts of the month's length (January, February, etc.) with 12-hour time step within a month. Thus, the data for the same name month for 56 year is separately considered. Splitting data in time by monthly intervals provides a compromise between information comprehensiveness and efficiency of computations. Moreover, it is convenient for the content analysis and organization of the modeling scenarios. Retention of time dependence in the inner structure of the input vectors and, hence, in the basis subspaces, gives a new facility and allows the time-dependent scenarios to be designed.

Thus, we have seven parameters to characterize each element of the database (4.4), (4.5). The first three of them are the ordinal numbers of the year, the month, the data field in terms of the physical content. The last four parameters define the space-time coordinates of data on the globe or its part: latitude, longitude, height, and time.

In terms of (4.5), the year number is the index- parameter $i = \overline{1,n}$, where n is the number of years in the database. The last five parameters set the internal structure and arrange the multi-index k in terms of (4.5),(4.6). The name (number) of the month is used as an input (dumb) parameter of the algorithm. It should be noted that the efficient computations might be organized for all the months' names in parallel .

Now the internal structure will be described. The size of the vector-columns of the matrix Z is defined by the following parameters. In terms of time, it is $2m$ (m is the number of days in a month, the fields are taken twice a day). The number of grid points in space , $144 \times 72 \times l$, presents the global domain in spherical coordinates with resolution of $2{,}5^\circ \times 2{,}5^\circ$ for the horizontal variables multiplied by the number of vertical levels , $l \geq 1$, parametrically given. The number of different physical components (≥ 1) is also introduced parametrically.

As the result of decomposition, the basis set of 56 elements (subspaces) is built. In all, there are 12 such sets of the factor spaces in accordance with the number of months in a year.

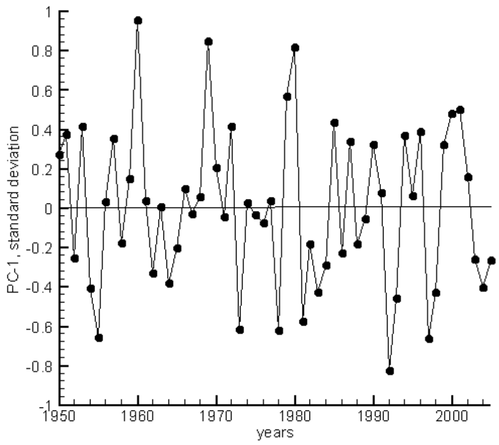
Thus, the long-term variability of the elements of the climatic system is presented by the structure which has two scales in time and uses the orthogonal spaces of two types. The first one is presented by the PCs, i.e. by the vectors $\mathbf{v}_q$, that characterize the year-to-year variability in the range of the external time scale. Their components $v_q(\beta)$ are the functions of the current number of the year β in the aggregate (4.5). The second type consists of the multivariate OBVs $\mathbf{\Psi}_q(\mathbf{x},t)$ dependent on the variables $(\mathbf{x},t) \in D_t^h$, where t is a local time within the monthly interval.

First of all, to analyze the long-term climatic tendencies, it is worth considering the predominant PCs and OBVs corresponding to $\lambda_q > 1$. The information content of the PCs and OBVs corresponding to $\lambda_q \approx 1$ is equal to that of the normalized deviation vectors of the input aggregate (4.5). The PCs and OBVs corresponding to $\lambda_q < 1$ can be considered as climatic and/or weather noises in the total information flow. They might be filtered out excluding the terms in the sum which are

associated with the small values of λ_q. In essence, each OBV is a multi-component subspace, the elements of which depend on the space coordinates and time within the month.
The merits of representation of the functions (4.5) as the orthogonal subspaces set are obvious. This is the usability of projecting the state functions onto OBVs and PCs and constructing the new subspaces with desired properties by means of linear combinations of OBVs. As the spaces are orthogonal, the total variance of the entire set is the sum of variances of all subspaces without interactions among them. Therefore, as it was mentioned above, the designed subspaces can be ranged with respect to the level of their significance.
The simultaneous analysis of the (PC, OBV)-pairs for different months shows the year-to-year and seasonal variability within the long-term interval. Analyzing the system $\left\{\mathbf{v}_q, \mathbf{\Psi}_q(\mathbf{x},t), q=\overline{1,n}\right\}$ jointly, one can notice that, in accordance with (4.9),(4.10), there are domains in which the components of OBVs have the maximal modules. They seem to pretend being the centers of energy activity in the climatic system. Remember, that here the energy is meant in the sense of the inner product (4.6).
Thus, using the results of orthogonal decomposition, both a quantitative and qualitative analyses of the complicated dynamic system behavior can be performed. Besides, the scenarios based on the prescribed criteria for solving diagnostic and prognostic problems can be deliberately formed.

5.2. Climatic data analysis and studying the climatic centers of activity

Since the middle of the last century, the research has been intensively performed on revealing and studying the climatic centers of activity in the atmosphere and ocean to define the most significant patterns having the prediction character. These regions on the globe where the relatively stable characteristics of the general circulation of the atmosphere exist, are usually referred to as such activity centers. They are, for instance, the quasi-stationary zones of high and low atmospheric pressure. Firstly Teisserence de Bort (1884) defined the concept on activity centers of the atmosphere. Since then, some areas of the sufficiently stable localizations have been described in the synoptic meteorology (see, for example, Zverev, 1968).
In the 80th years of the last century G. Marchuk considered a concept of the energetically active zones of the ocean which are characterized by increased energy releases from the ocean to the atmosphere (Marchuk et al. 1984). In frames of the concept, the studies of the activity zones for the goals of weather prediction were fulfilled with the use of the theory of adjoint equations (Marchuk, 1974).
The methodology proposed here gives the possibility to quantitatively examine the hypotheses on existence of energy active zones in the atmosphere and ocean and to study their spatial-temporal variability as manifestation of the dynamic system evolution in the phase spaces with the basis of PCs-OBVs.Now we shortly present some results of analysis of the climatic system behavior for 56 years (1950-2005). For the longest months of 31 days, as many as 3472 fields for each state function have been used.



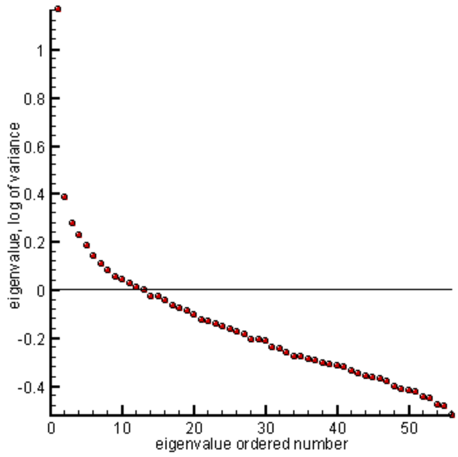


Fig. 5.2.1. *Time variation of the leading PC-1 for the 500-hPa geopotential height for January (1950-2005).*

Fig. 5.2.2. *Eigenvalues of the Gram matrix for the 500-hPa geopotential height for January (1950-2005).*

The time behavior of the leading PC-1 for January of many years is shown in Fig. 1. It is calculated for the 500-hPa geopotential height. Circles show the values (standard deviation, $\sigma_1 = \sqrt{\lambda_1}$) of the PC-1 components corresponding to the year number. The scale of the vertical axis is defined by normalization from (4.8). The components of the PC-1 reflect the relative input of each generalized January field into the leading factor space OBV-1. The years in which the absolute values of the component PC-1 are greater, give the greater input in the OBV-1.
In Fig. 5.2.2, the eigenvalues (4.8) of the Gram matrix Γ are shown in descending order. The vertical scale is defined by the value of the Gram matrix trace which presents the total variance equal to 56. The logarithmic scale of the vertical axis is chosen in Fig. 2. The first eigenvalue is seen to be strictly dominated. It gives the input of 26,34% into the total variance of the whole set. The leading PSs and OBVs with numbers from 1 to 13 hold the information in the climatic sense: the corresponding eigenvalues are greater than 1. These 13 informative PCs and OBVs accumulate more than 50% of the total variance. Exactly these components can serve as the base for the climatic scale behavior description. The horizontal line in Fig. 3.2 separates them from the other eigenvalues mentioned above as presenting the climatic and /or weather noises.
In Figs. 5.2.3-5.2.6, the fragments of the leading OBVs corresponding to the maximum eigenvalues of the Gram matrix for the 500-hPa geopotential height for 56 years are presented for four months, one for each season. Each vector OBV presents the subspace that consists from $2m$ such fields in time, where m is the number of days in a month. Remember that the OBVs are normalized as in (4.8). The fragments are taken at 00:00 UTC on 15 January (Fig. 5.2.3), 15 April (Fig. 5.2.4), 15 July (Fig. 5.2.5), and 15 October (Fig. 5.2.6) , respectively. In Figs. 5.2.3.-5.2.7, the vertical axis shows the function of latitude so that the South Pole is 0° and the North Pole is 180°. The horizontal axis is the longitude starting from the Greenwich meridian. The continents' configurations are marked by the thick lines. Regions of local maxima and minima can be interpreted as centers of activity or energy active regions. Analyzing the temporal behavior of the OBVs-1 for different components in different months, we can conclude the following. The space structures in the OBVs-1 are of the global scale. Their behavior can be classified as quasi-stationary because their geographical locations change insignificantly within the month. In the high latitudes of the Northern Hemisphere, in January, and in the South Hemisphere, in June, they are more stable than in the transition periods. The intensity of perturbations and the scales of domains of their carriers decrease in autumn and spring. The contrasts in the character of the circulation mechanisms in the

high latitudes of the both hemispheres become less pronounced. With the increase of OBV's number, the amplitudes of perturbations decrease and the patterns of the small-scale structure manifest themselves (not shown here).

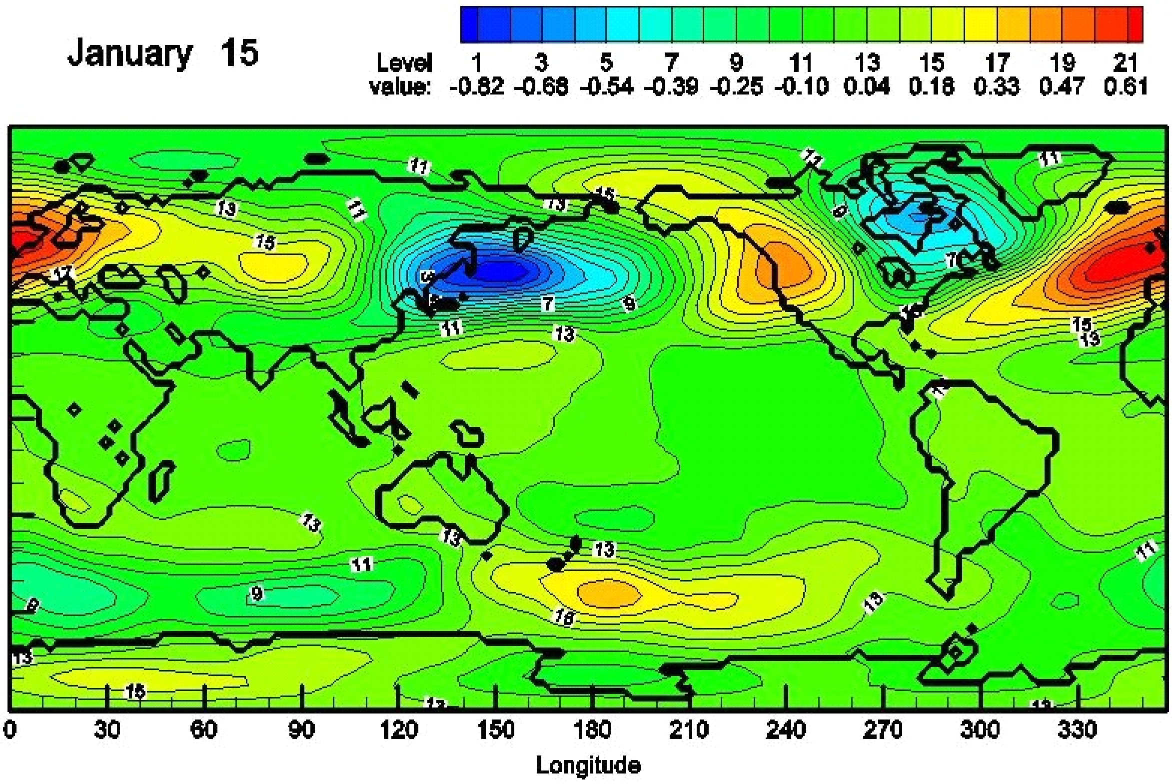


Fig.5.2.3. *One of the 62 fragments of the leading OBV-1. The basis is constructed on reanalysis data of the 500-hPa geopotential height for 56 years. The fragment corresponds to 0000 UTC 15 January.*

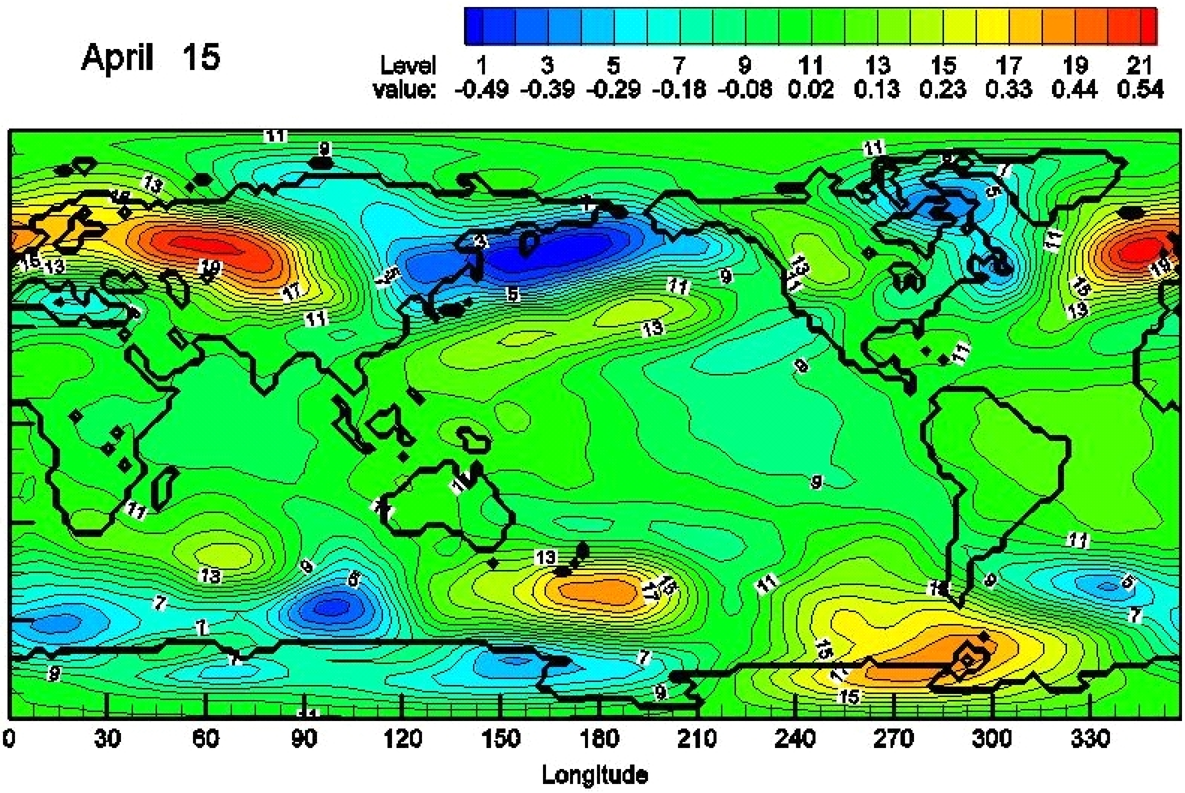


Fig.5.2.4. *The same as in Fig. 3 but at 0000 UTC 15 April.*

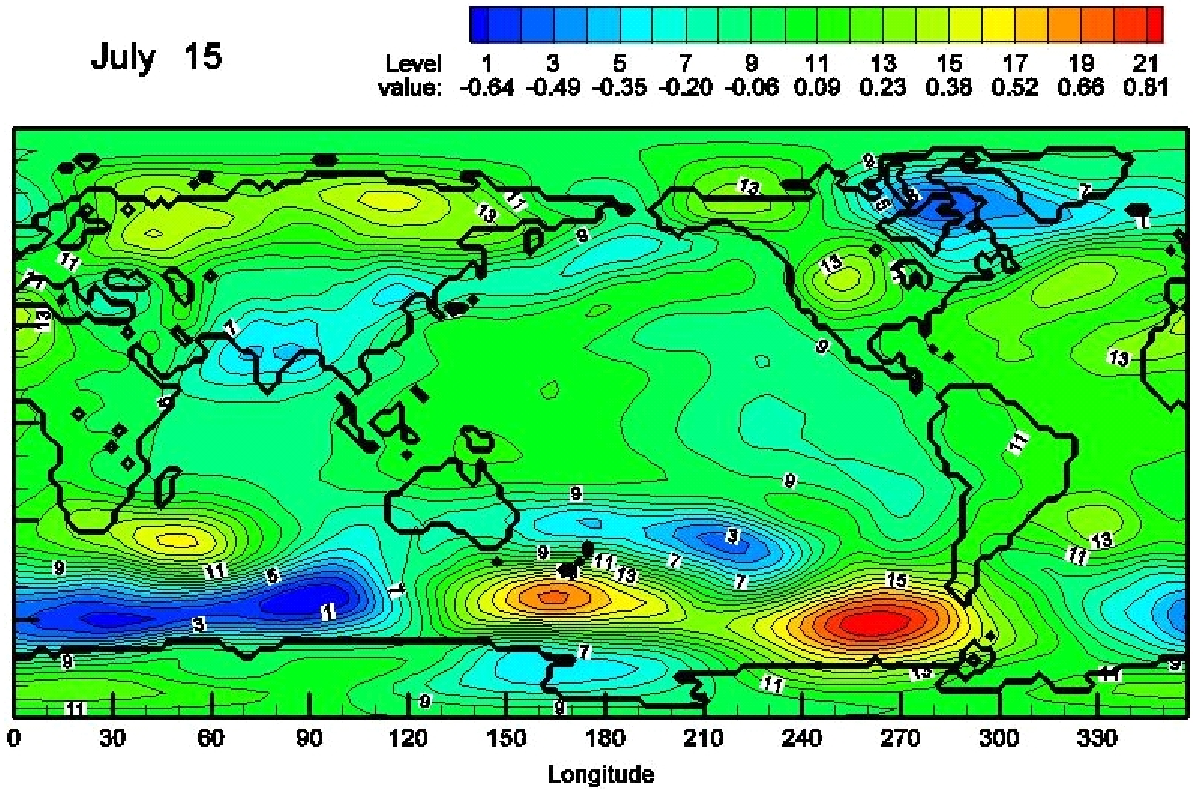


Fig.5.2.5. *The same as in Fig. 3 but at 0000 UTC 15 July.*

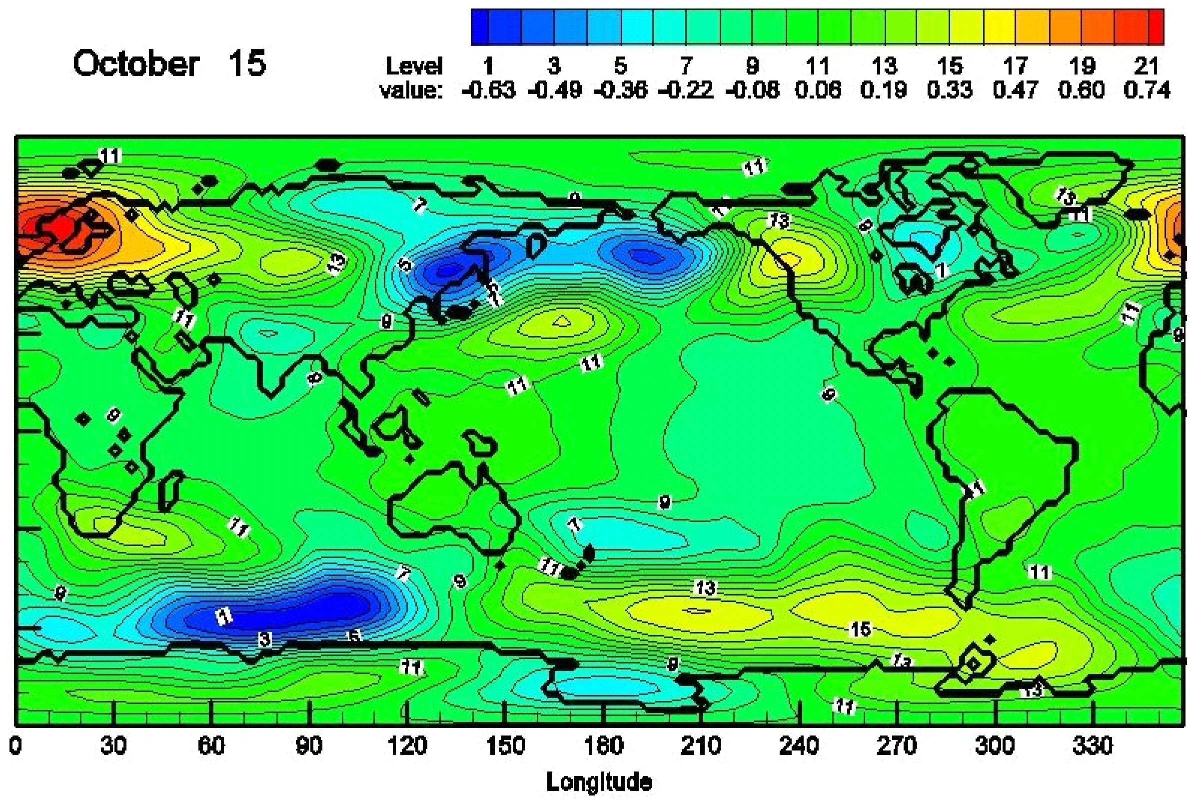


Fig.5.2.6. *The same as in Fig.3. 3 but at 0000 UTC on 15 October***.**

In Fig.5.2.7, one of the 62 fragments in time of OBV-1 for January (1950-2005) for the velocity component is demonstrated. It corresponds to the fields of the horizontal components of the wind velocity at the level of 500 hPa. In January, the circulation above the continents in the Northern Hemisphere is caused by the competition between the Pacific and Atlantic Oceans. The circulation structures over the Eurasia are separated near the meridian of 100° E (compare with Fig.5.2.3). In

July the summer type of circulation is characterized by latitudinal character (Fig.5.2.5). It should be noted that the leading space OBV-1 for velocities is quasi-stationary during the month as it is for the geopotential height. The main circulation systems have the sufficiently stable localization in the space as well.

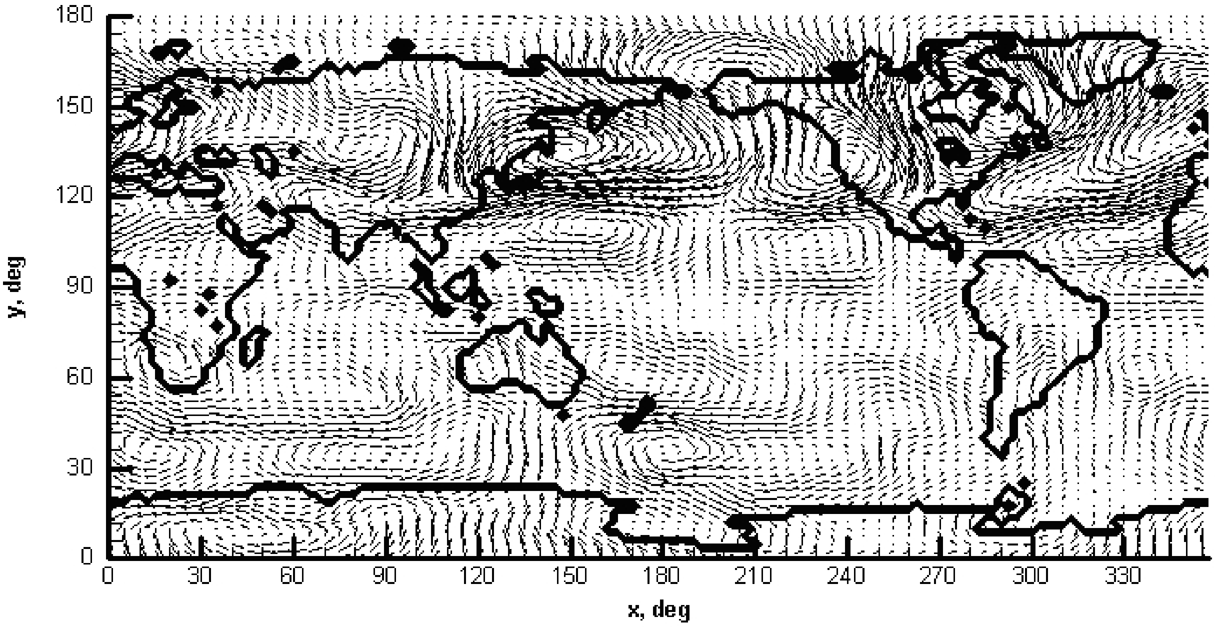


Fig.5.2.7. *One of the 62 fragments of the leading OBV-1. The basis is constructed on reanalysis data for horizontal wind components at 500-hPa level for 56 years. The fragment corresponds to 0000 UTC 15 January.*

Fig.5.2.8 shows the seasonal behavior of the information index μ_1 (%) of the first leading pair (PC-1,OBV-1) with respect to the total variance of the systems presenting the subsets of reanalysis data for each of 12 months. In this case it is the energy of perturbations in the sense of (3.1). It is seen that the seasonal behavior has two local maxima. The greater one is related to the winter month, the lesser one is related to the summer month. As the seasons in the Southern and the Northern hemispheres are opposite, the difference in the intensity of maxima can be explained by the fact that the land-ocean contrasts manifest themselves more brightly in the Northern hemisphere.
The same characteristics of decomposition were early calculated for the period of 40 years (1960-1999) (Penenko and Tsvetova, 2002, Penenko and Tsvetova, 2003). Comparing the configurations of the first leading vectors for the periods of 40 years with those of 56 years, we can conclude that the number of activity centers keeps to be the same . Their geographical locations did not change, either. Thus, there is no essential reconstruction in the leading basis vector when the total number of the input vectors is significantly increased.

Summarizing, we can repeat that the leading OBVs have a relatively high information significance and they are quasi-stationary. More over, 10-15 of them contain more than 50% of the total variance of the system. Hence, it can be concluded that the system possesses a long-term deterministic memory. This fact may serve as an argument for the validity of the hypothesis of relative stability of the climatic background which is described by the leading PCs and OBVs. It should be mentioned that this conclusion is made when the concrete database is used and the concrete structuring is chosen. Nevertheless, the designed bases seem to be useful for the construction of guiding phase spaces for the goals of long-term environmental prediction, design and ecology studies.

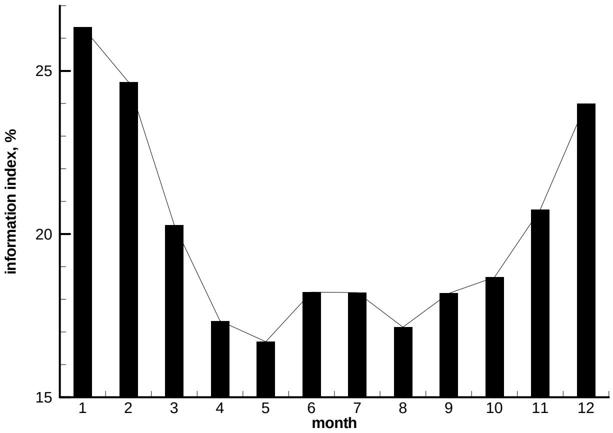


Fig.5.2.8. *Seasonal variability of the information index* μ_1 *(%) of the leading pair (PC-1,OBV-1).*

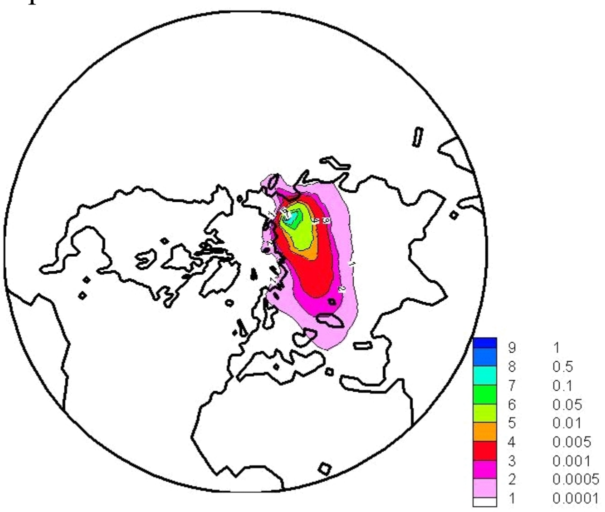
5.3. Principle factors and Siberian regions

The Siberian regions are of special interest for us from the viewpoint of decomposition of circulation mechanisms and their manifestation in the formation of environmental dynamics.
Joint analysis of basic subspaces, the fragments of which are presented in figs. 5.2.4-5.2.7, shows that Siberia and especially the Lake Baikal region are situated in the places which separate the circulation systems of high energy activity. In winter season they are between the Pacific and Atlantic energy-active zones whereas they separate the Arctic and South-Asian zones in summer seasons. These facts may explain high dynamic activity in the region. In the autumn-winter season the instability expresses as sharp alteration of weather cycles. The formation of Altai-Sayan cyclogenesis which is of the same intensity as the Mediterranean one, is specific for warm seasons. In works (Chung et al. 1977, Chen et al. 1991) it is referred as lee-type cyclogenesis. This is the large scale phenomenon in the climatic system of the central part of Eurasia. Its influence is represented in the environmental dynamics.
The region of Lake Baikal falls into the zone which is characterized by the high degree of cyclone activity and therefore is situated on the cross-roads of air pollution transport. The observing system which are in Siberia shows that man-made emission leads to the worsening the air quality. The typical sources of emission having influence on ecological situation are the following: industrial objects on mining and making of mineral resources and energy production, vast forest fires, etc. In the recent years the emission of aerosols stimulated by military conflict in Afghanistan and Irak, dusty storms in the Central and South-East Asia was increased. Due to the climate change in Western Siberia the methane emission from the wet soils and wetlands became stronger. As a result of photochemical reactions, the increased concentrations of formaldehydes and other active products are produced.
This creates the pre-conditions for arising the situations of ecological risks and demands of particular attention to the planning of economic activity and environmentally protected strategies in the region. From the point of view of system analysis, the methods of orthogonal decomposition along with the methods of sensitivity theory and risk assessment offer a tool which allows one **to move the results of the global atmospheric and climatic studies onto the regional level.** Namely this level puts the concrete questions on the environmental quality and its changes.

5.4. Risk assessment and observability of territories with AEROSIBNET

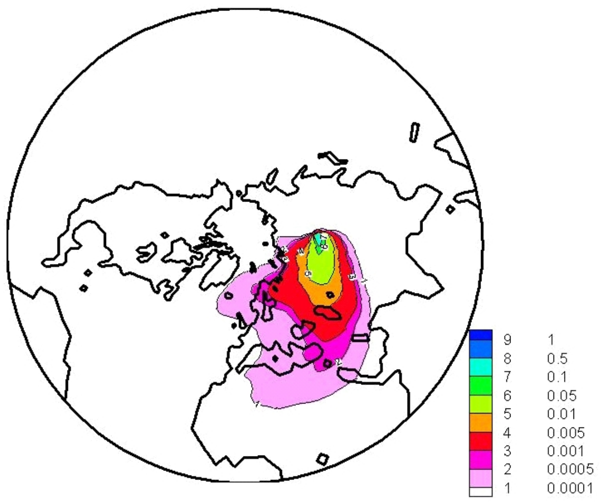
Let us consider an example of modelling scenario showing some applications of the presented variational methodology, in particular for: 1) estimation of risk and vulnerability of territories; 2)

estimation of observability of territories by means of a monitoring system and solution of inverse problems; 3) identifying sources by inverse modelling.
The Siberian part of the global observational system AERONET (Holben et al., 1998, Sakerin et al., 2005) is of great interest in this context and can conveniently be used for this task. Some features of AEROSIBNET (Sakerin et al., 2005) are taken into account for the choice of receptors and formation of target functionals. Nine industrial Siberian cities from the Ural mountains up to the Pacific Ocean containing aerosol monitoring stations are taken as the receptors for risk assessment.
The ground-based stations equipped with sun/sky photometers are the basis of the monitoring network. They measure vertically integrated optical spectral properties of the atmosphere and the concentration of aerosol particles as a function of size. To describe these integrated data we define functionals of the type of Eq. (2.8) which contain both the corresponding model of observation in the form of Eq. (2.4) and the weight functions showing the position of monitoring devices in time and space.



(a) (b)

Fig.5.4.1.*The sensitivity functions (reference values) for monitoring stations placed in Yakutsk (a) and in Ekaterinburg (b).*

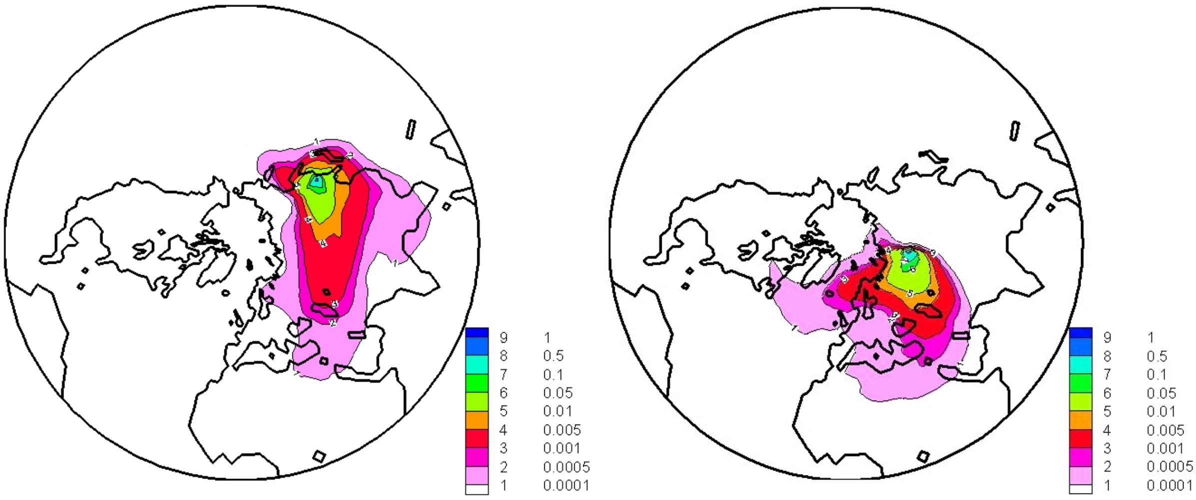


(a) (b)

Fig. 5.4.2. *The sensitivity functions (reference values) for monitoring stations placed in Mondy (a) and in Khanti-Mansiisk (b).*

The variational principle for studying the target functionals with the use of the models of transport and transformation of aerosols and the SFs gives the scan-out of the information incorporated in target functionals in the phase space. It enables to develop effective procedures of data assimilation

for the estimation of atmospheric conditions, for estimation of risks/vulnerability and for the organization of control strategies.
The realization of scenarios is carried out employing a system of global models of chemical tracer transport in the atmosphere (Penenko and Tsvetova, 1999). The models are used in forward and inverse modes within the frame of the basic algorithm (items (**1**)-(**4**)). The atmospheric circulation was simulated using NCEP/NCAR reanalysis data (Kalney et al., 1996) and our dynamical model (Penenko and Tsvetova, 1999a). Fast data assimilation procedures (Penenko and Tsvetova, 2002) were applied in the model with 20 levels in the vertical. A time step of 30 minutes was used.
Results derived for this scenario are presented in Figs. 1-6. The sensitivity-risk-observability functions are shown in Figs. 5.4.1-5.4.3 for six monitoring stations (from nine) placed in the receptor area.

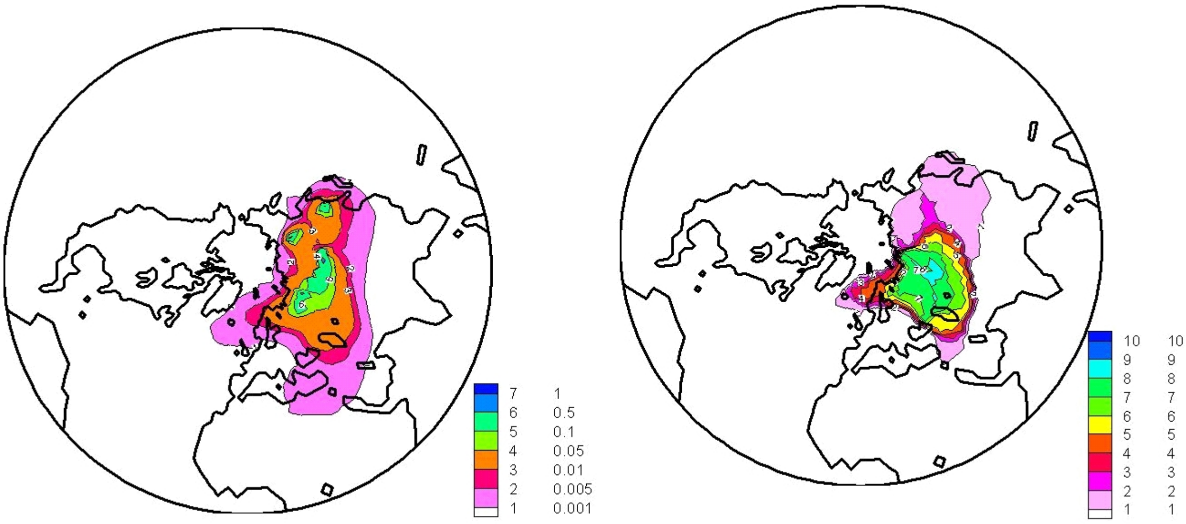


(a) (b)

Fig. 5.4.3. *The sensitivity functions (reference values) for monitoring stations placed in Ussuriisk (a) and in Tomsk (b).*

The territory is considered as an observable one for a monitoring station if it is met by the carrier of the sensitivity function for this station. The risk function for a receptor in relation to sources coincides with the function of observability. Figure 5.4.4a gives the function of total observability of the territory by means of these 9 stations in relation to the ground sources of pollution. In Fig.5.4.4b the location function of sources of aerosols derived from the data observed in the receptor area is presented. The location function of sought sources is formed from overlapping of the carriers of the sensitivity function for separate functionals. The function shows the number of monitoring stations which can observe the same area. The values of this function are the sum of the characteristic functions constructed for each observability function. There are 9 stations in our scenario. It means that integer-value location function can vary from 0 to 9. The areas with the highest level of the significance have to contain the sources. Most probably these sources released the aerosols which were measured by these stations.
Thus the proposed way of treating observational data allows one to get the estimations of risk/observability domains of large extension. This is due to the fact that propagation of information from vertically integrated functionals to space-time domains is carried out in the frame work of inverse modelling.
If AERONET is used in such an approach, it is possible to get information about the sources of pollution from large territories. This is especially important for the northern regions and Siberia where regular observations of environmental quality are hard to achieve.
The main factors which are discovered in the behavior of the state functions by means of the orthogonal decomposition methods, show the dynamically and energetically active zones in the climatic system. The principle component analysis for sensitivity functions gives the possibilities for revealing the regions of the increased ecological risks and vulnerability. It is naturally to expect

that the energy active zones and those of the increased ecological risk are in close connection. The figures presented demonstrate such relations. For example, the monitoring station near Ussuriisk, which falls into the Far-East energy active zone, has the most spacious sensitivity/ observability function as compared to the other monitoring sites.



(a) (b)

Fig. 5.4.4. (a) The function of total observability of territories by means of nine monitoring sites. (b) The location function of sources which could release the aerosols observed by all the measuring sites.

If the locations of the monitoring station is treated as receptors, in which the atmospheric quality is measured by remote methods, then the SFs show the territory where the pollution may come from into this receptor. The quantitative estimates of the functions define which portion of the total emission from the sources, placed in the observability domain, may obtain the receptor. That is what the quantitative risk/ vulnerability assessment with respect to the sources. Thus, SFs demonstrate the multi-goal character of such analysis.

5.5. Applications of forward and inverse techniques for risk assessment in Siberian region

This part is shortly describes some findings of the SB RAS interdisciplinary project "Ecological problems of Siberian cities". The partner ICMMG was one of the coordinators and executors of the project which concerns with urban problems for typical Siberian cities. The representatives from twelve scientific institutions of SB RAS as well as the colleagues from non-academician organizations took part in it. The goal of the project was to fulfill the multidisciplinary studies which can help to clarify the questions: how do cities change hydrodynamic behavior and composition of the atmosphere and how do these changes affect the quality of life, public health and quality of environment?

The fundamental aspects were considered and some measurements were made that connected with diagnosis and forecast of environmental quality. Each scientific area used its own methodology. To integrate the knowledge from different disciplines, information and modeling technologies were used. The methodology of adaptive and targeting observations was realized in several complex observational experiments for monitoring environment conditions in the cities Irkutsk, Angarsk, Usolye-Sibirskoye, Tulun, Nizhneudinsk, Taishet, Kansk, Krasnoyarsk, Achinsk, Tomsk, Novosibirsk, Ulan-Ude, Norilsk. The analysis of the results has shown the presence of both the common and specific features in hydrodynamic circulation and distribution of pollutants in the atmosphere of Siberian cities.

For Novosibirsk city and region the monitoring of the atmosphere are supplemented by a complex of the studies of the snow cover, soil, and biotopes in places with various levels of man-made

load. The microbiological studies of the air, ground, snow, leaves of trees have also been done. As addition to the atmospheric measurements the maps of spatial distribution and the biochemical state of the lichens in Novosibirsk region were drawn. The lichens accumulate the long-term pollution and therefore can be considered as an indicator of the pollution level.
For various cities of Siberia, the estimations of erythema levels and variability of intensity of ultra-violet radiation of the Sun were produced. The UV radiation impacts on parameters of health and ecosystem efficiency and influences on the mechanisms of pollutants' transformation in the atmosphere.
Further some examples of numerical scenarios for Siberian Federal District (SFD) calculated by the ICMMG team are given. The methodology of environmental modelling described above are essentially used in them. The ecological risks connected with an exchange of pollution between the large cities are given in Fig1. In this scenario, calculated forward in time, the cities are considered as aggregated sources. It should be noted that we need the emission data to calculate the fields of concentrations and risk assessment.
The risk scenarios calculated by means of regional numerical models in the inverse mode do not demand such data for realization of scenarios and risk assessment. Here the cities are considered as receptors and the goal functionals of atmospheric quality in receptors are introduced. In Figs. 2-3 the risk functions for the cites to get pollution from the acting and potentially possible sources, placed at the surface layer, are presented. The instant snapshots of the risk functions show configuration and relative input of the regions, the emission from which can influence on the atmospheric quality in the receptors. Such data are more informal then those of forward scenarios for the decision-makers, because the role of each source (separately) are seen whereas the forward scenarios give the summarized effect of all sources.

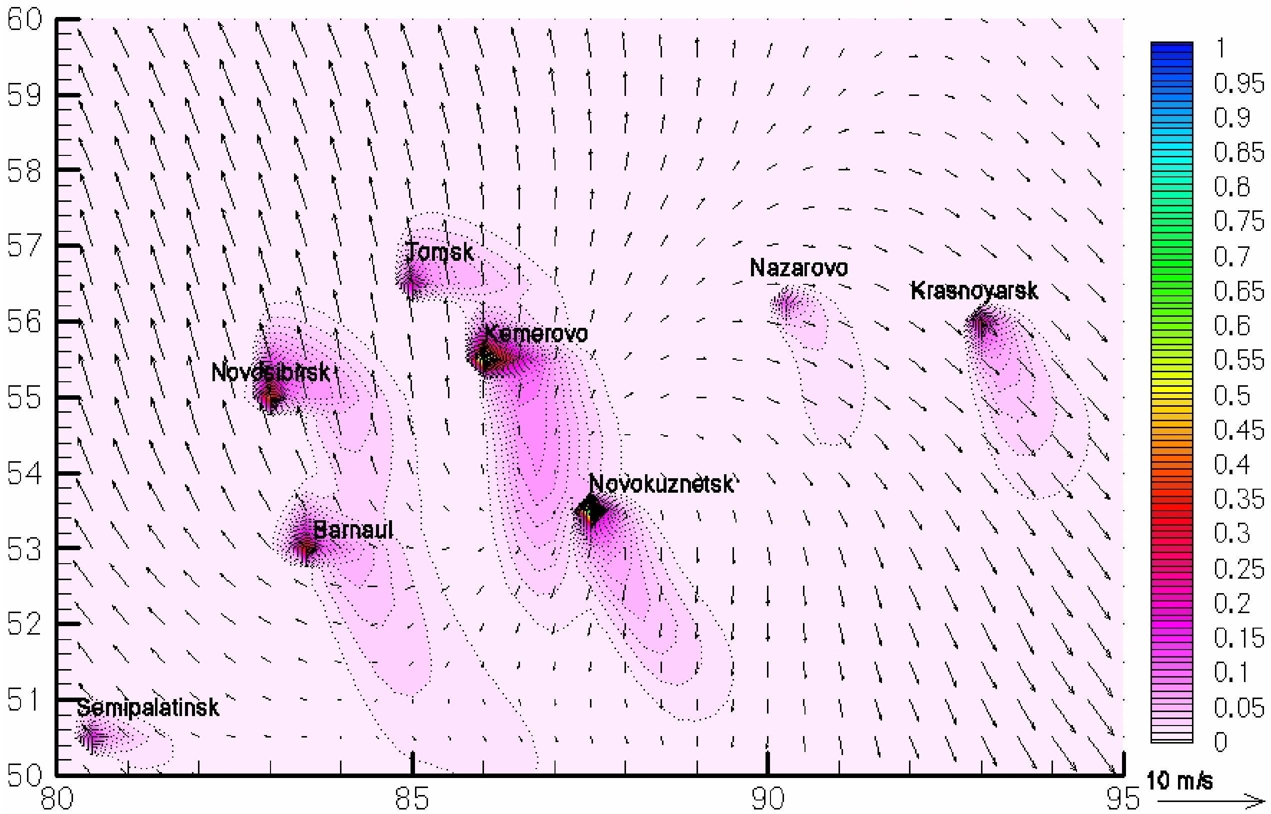


Fig.5.5.1. *Pollution of the atmosphere in Siberian Federal District. Big cities are considered as aggregated sources of pollution. Surface layer. Fragment of the forward scenario. Hydrodynamics is reconstructed by means of the regional model taking into account the global circulation /arrows show wind field (m/s)/*

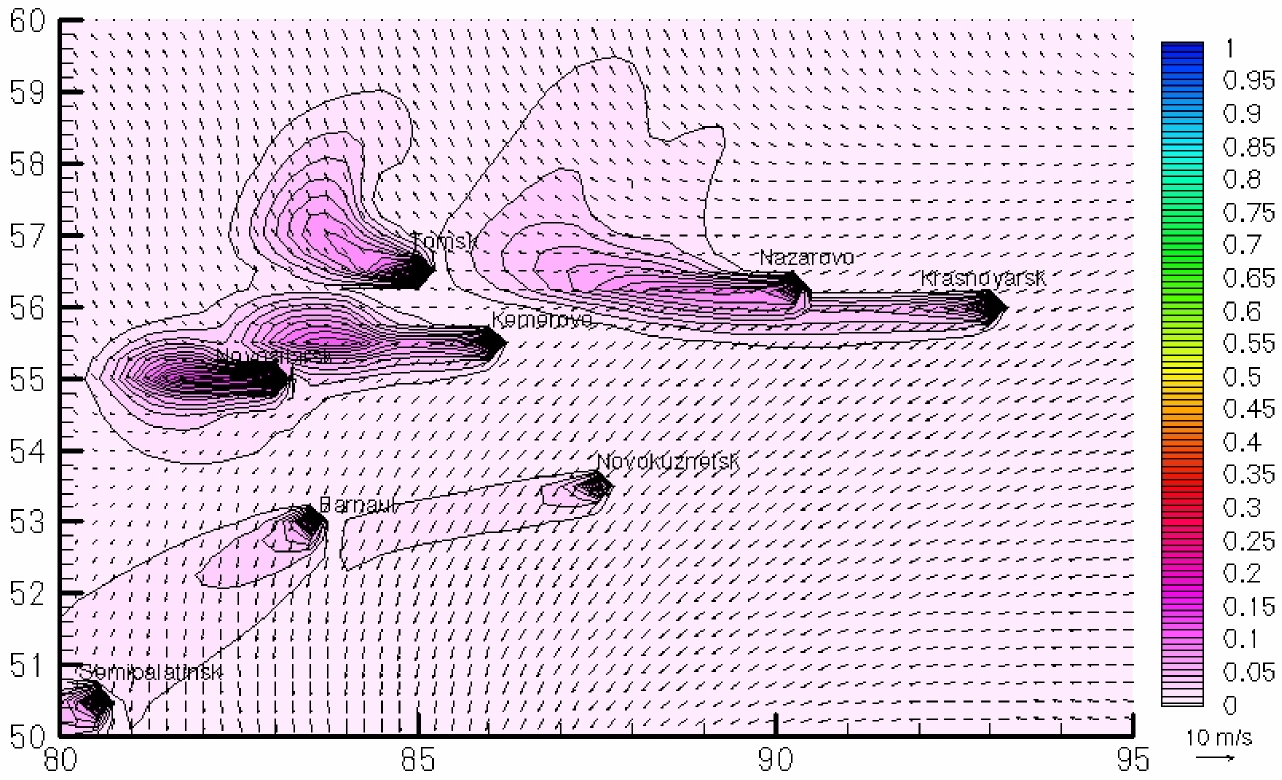


Fig.5.5.2. *The fragment of the 4D risk function (relative units) and velocity vector (m/s) for the moment 11:30 12/06/2002 for the cities of Siberian Federal district. Surface level.*

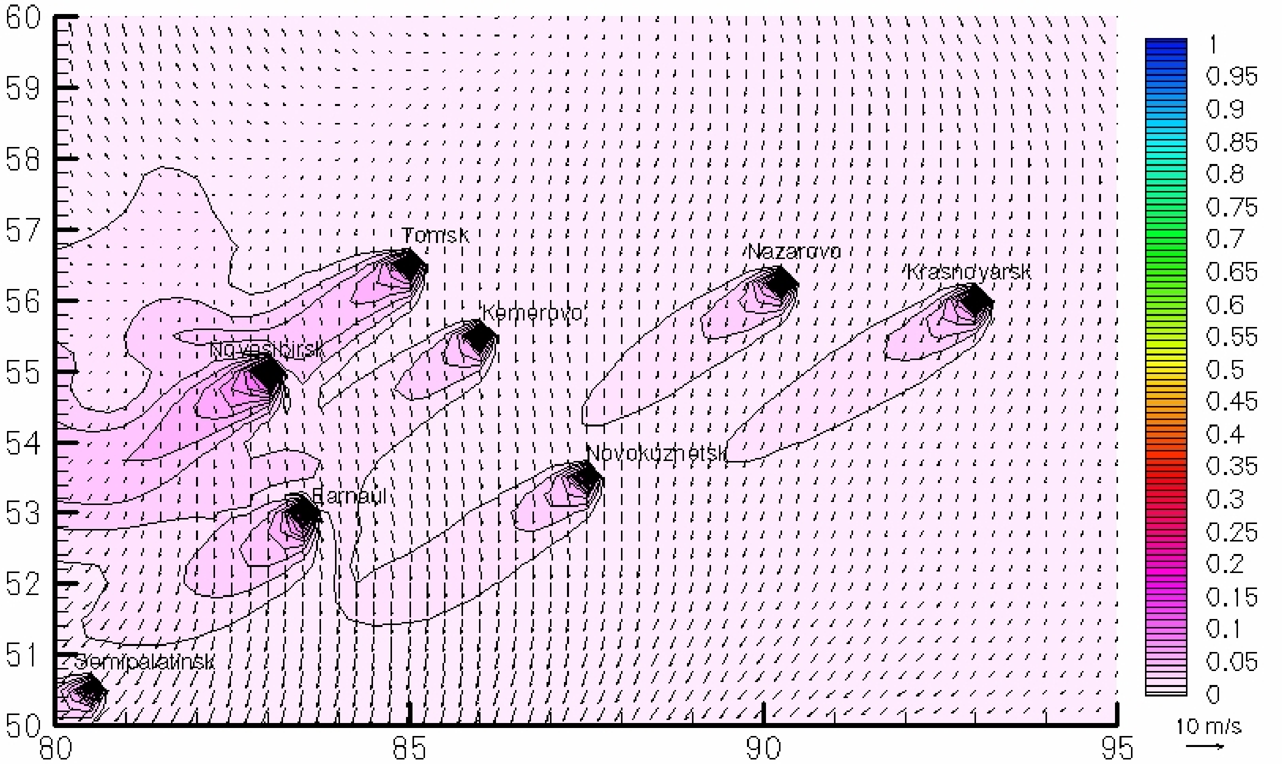
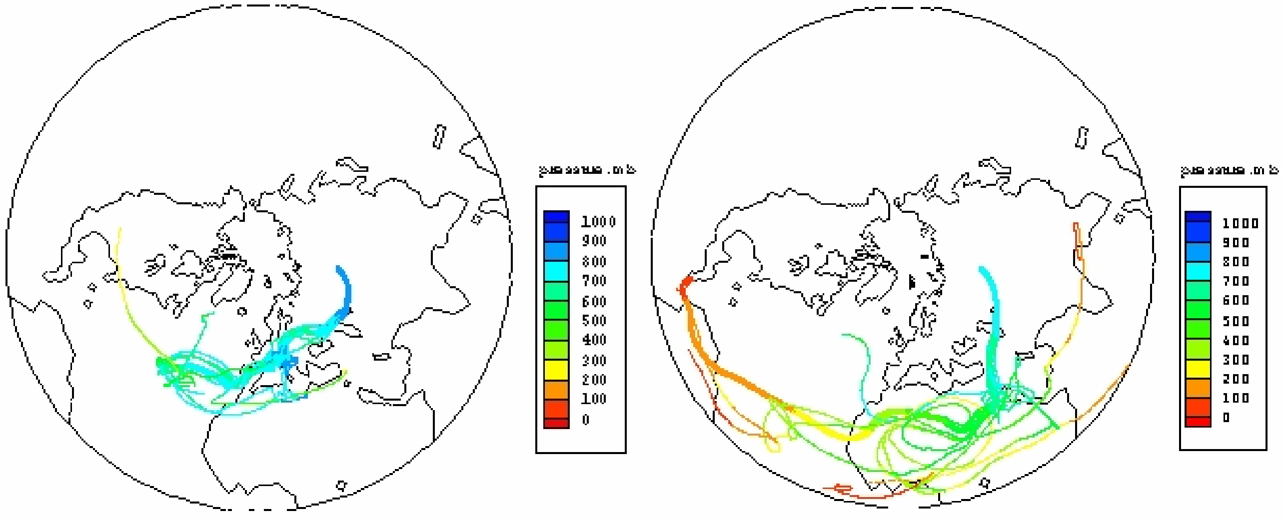


Fig.5.5.3. *The same as in Fig.5.5.2, but for the moment 8:20 11/06/2002.*

The scenarios of possible traces of active bioaerosols into Novosibirsk region were calculated as well (Figs. 5.5.4-5.5.6). The problem was formulated for interpreting the data obtained in the measurements made by the aircraft monitoring system of IOA SB RAS. The data were treated in the laboratory of the State Virology and Biotechnology Center “Vector”. Both of the institutions were the partners in this project. Two types of inverse scenarios were made for this goal. The adjoint sensitivity analysis was made for Lagrangian and Eulerian variational frameworks for the same quality functional, time intervals and meteorological situations.



(a) (b)

Fig.5.5.4. *(a) Adjoint backward trajectories show possible pathways of bioaerosols to the atmosphere of the receptor above Novosibirsk city. Receptor's coordinates (54.24 N , 82.09 E), pressure level 850 mb. Deterministic-stochastic particle transport model in Lagrangian framework and (b) The same as in Fig 5.5.4, but for receptor's pressure level 700 mb.*

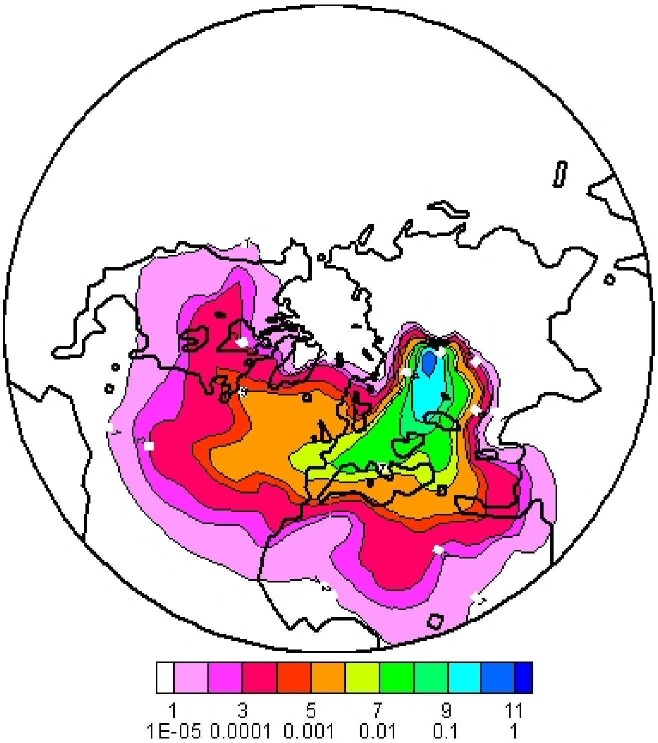


Fig.5.5.5. The 2-D cross-section of the risk/observability function (normalized) for Novosibirsk as the receptor. Inverse scenario for transport model in Eulerian framework.

Fig.5.5.4. Adjoint backward trajectories show possible pathways of bioaerosols to the atmosphere of the receptor above Novosibirsk city. Receptor's coordinates (54.24 N , 82.09 E), pressure level 850 mb. Deterministic-stochastic particle transport model in Lagrangian framework. In this figure the adjoint backward trajectories calculated with the help of adjoint mode of the deterministic-stochastic particle transport model in Lagrangian framework are shown. Height (pressure level in mb) of trajectories is indicated by the colors according to the scale. A result of the adjoint inverse scenario in the transport model in the Eulerian statement is presented in Fig 5.5.5. The function shows relative degree of influence of the sources placed in the surface level on the quality of the atmosphere in the receptor.

5.6. Assessment of the influence zone of Boguchan reservoir and unfrozen patch of water in the tail-water of hydropower plant on the ambient atmosphere

This is typical for many cities that they are located near the rivers or water reservoirs. In Siberia conditions this implies the formation of the specific mesoclimates which stimulate the accumulation of pollution in the surface layer in the conditions of predominantly stable stratification of the atmosphere.
The goal of the study is to estimate the possible changing the regional climate connected with the projected Boguchan power plant and the artificial reservoir near it. The project is realized in the Siberian Federal District in Krasnoyarsk and Irkutsk regions. The Boguchanskaya hydropower plant is the forth in the cascade of the hydro plants on the Angara river.
The planned basic parameter of the project are the following:

- normal supporting water level - 208m
- reservoir volume-52,8 km^3
- length of the reservoir –375 km
- area of the water mirror –2376 km^2
- flooded area – 1494 km^2
- maximal width – 14-15 km
- minimal width about 1,2 km.

The appearance of such big water body will remarkably change the thermodynamics properties of the underlying surface in the region. This, in turn, will entail some consequences in mesoclimate of the territory.
The govern system of the mesoscale model of atmospheric hydrodynamics includes the equations of motion, heat, humidity and continuity in the form

$$
\begin{aligned}
&\frac{\partial \rho u}{\partial t} + div\,\rho u\vec{u} = -\frac{\partial p'}{\partial x} + l\rho v + \Delta_u u\ ,\\
&\frac{\partial \rho v}{\partial t} + div\,\rho v\vec{u} = -\frac{\partial p'}{\partial y} - l\rho u + \Delta_v v\ ,\\
&\frac{\partial \rho w}{\partial t} + div\,\rho w\vec{u} = -\frac{\partial p'}{\partial z} + \lambda\rho\vartheta' + \Delta_w w,\\
&\frac{\partial \rho \vartheta'}{\partial t} + div\,\rho \vartheta'\vec{u} = -S\rho w + \rho\frac{L_w}{c_p}\Phi + \Delta_\theta \vartheta'\ ,\\
&\frac{\partial \rho q'}{\partial t} + div\,\rho q'\vec{u} = -\rho w\frac{\partial Q}{\partial z} - \rho\Phi + \Delta_q q',\\
&div\,\rho\vec{u} = 0.
\end{aligned}
$$

Here t is time, $\vec{x} = (x, y, z)$ are Cartesian coordinates, $\vec{u} = (u, v, w)$ is wind velocity vector, ϑ', q', p' are the deviations of the potential temperature, specific humidity and atmospheric pressure from their background values, $\rho = \rho(z)$ is the given atmospheric density, Q is background specific humidity, L_w is latent condensation heat, Φ is the rate of generation of the liquid phase, c_p is the specific heat at a constant pressure, l is Coriolis parameter, S, λ are parameters of stratification and buoyancy.
Operator Δ_α ($\alpha = u, v, w, \vartheta, q$) has the form $\Delta_\alpha = \frac{\partial}{\partial x}\mu_{\alpha x}\frac{\partial}{\partial x} + \frac{\partial}{\partial y}\mu_{\alpha y}\frac{\partial}{\partial y} + \frac{\partial}{\partial z}\nu_\alpha\frac{\partial}{\partial z}$, where $\mu_{\alpha x}$, $\mu_{\alpha y}$ $\mu_{\alpha z}$ are the coefficients of turbulent diffusion in x, y, z directions correspondingly.
Zero values for deviations of the meteo elements are taken as initial conditions for the problem. The boundary conditions are given in the following way: the Neumann conditions are set at the

lateral boundaries and the vanishing of the disturbances is assumed at the upper boundary. The orographic and temperature variations of the underlying surface are taken into account in the Robin conditions at the lowest model level which coincides with the upper boundary of the surface layer. The equations are integrated in the domain $D_t = D\times[0,T]$, where $D=\{0 \le x \le X,\ 0 \le y \le Y,\ \delta(x,y)+h \le z \le H\}$, and $0 \le t \le T$ is the time interval, h is the height of the surface layer, $\delta(x,y)$ is a function describing the relief of the territory. The temperature of the underlying surface and the solar radiation obtained by the Earth surface are calculated with the account of the inclination and exposition of the slopes.

The data SRTM, which are the simple 16-bit raster, are taken as initial topography data. The value of the pixel is the height of the relief in the point over the sea level. To provide the studies, the region of 280 km x 280 km was chosen. It completely includes the reservoir and the part of the territory from the tail-water side.

The meteorological characteristics with the help of which the background fields were constructed were taken for the Kejhma meteostation in the Krasnoyarsk region.
In this study we assess the influence of new objects on the distribution of the basic meteo fields such as temperature, wind and humidity. To this goal we simulate the mesoclimate of the territory for different seasons of a year. And two sets of numerical scenarios are fulfilled: the first case is without the reservoir and the second one is with the reservoir filled to the planned supporting level of 208 m.
The results of modeling are the 4D fields of wind velocity components, pressure, potential temperature and specific humidity. They reproduce the daily behavior of basic meteoelements in the conditions specific for each season. The differences between the corresponding cases give the possibility to assess the influence of the new objects.
In Fig. 5.6.1 the results for the summer period are presented. The cooling influence of the reservoir is strictly pronounced. The isoline of the temperature decrease on 0.1 degree separates 3-6 km distance from the coast. One can mark the local positive deviations of the temperature far from the shore line mainly over the high relief forms. The explanation of the fact can be the strengthen of the breeze circulation that promote the output of the warm near surface air up along the slope.

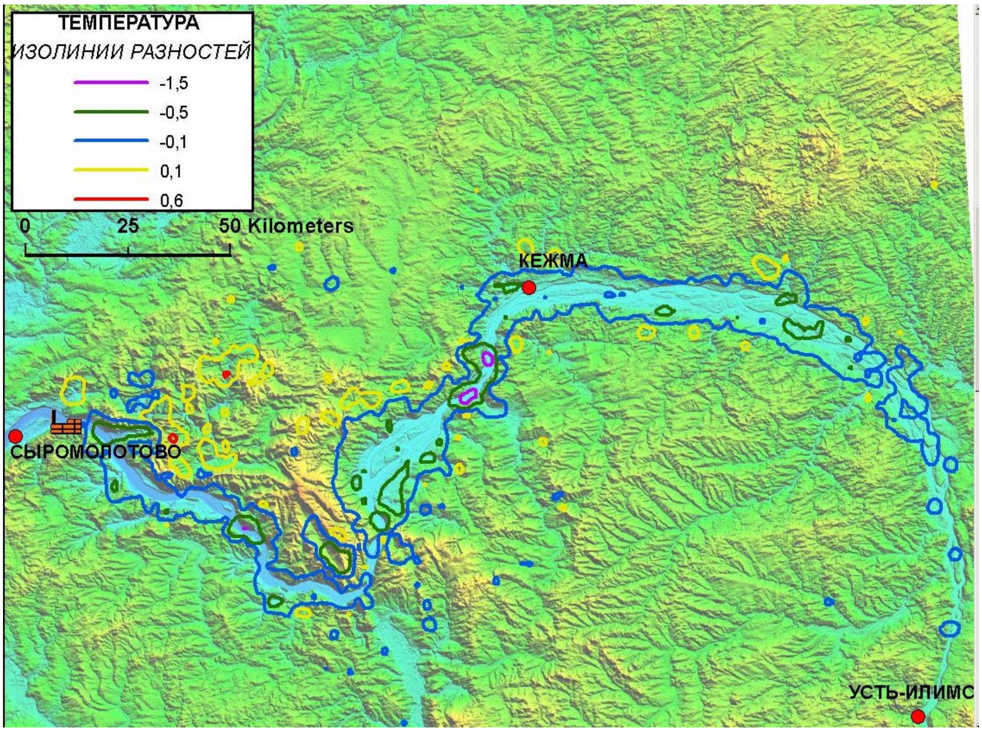


Fig.5.6.1. *Isolines of the temperature differences (deg. C) at the surface layer height in summer scenario.*

In the absence of the background flow the increase of the wind velocity on 0.2-0.5 m/s is obtained practically everywhere near the shore. The local maximums about 1 m/s are calculated. The distance of the breeze penetration is estimates by the 4-8 km from the shore. Any remarkable increase of humidity in the summer period was not seen in the calculations.
For autumn period the background flow of 1.5 m/s was prescribed. The increase of the upcoming flow was shown over the water surface which could be explained by the appearance of the additional smooth open surface of the reservoir. The influence of the reservoir is mostly pronounced in the lee side. In the day time the weak cooling effect of the reservoir is obtained. In reverse effect is shown in the night. The increase of the relative humidity is not big and mainly seen above the wide parts of the water surface.
In winter conditions the stable stratification of the background atmosphere was supposed. The water temperature of the unfrozen patch was 0˚C. The temperature of the air at the surface - 25˚C. In the numerical experiments the length of the unfrozen patch was prescribed as 45 km. In the absence of the background flow the atmospheric circulation forms mainly due to the temperature and topography heterogeneities of the underlying surface. The high banks and the absence of the background flow lead to the fact that the remarkable changes of the temperature and humidity concentrate within the 1-2 km distance from the unfrozen patch. The isoline of 1˚C -increase of the temperature is on about 1 km distance from the unfrozen patch (Fig. 5.6.2). The isoline of 10% increase of relative humidity at the height of 60 m from the surface is about 1-2 km from the patch (Fig.5.6.3).

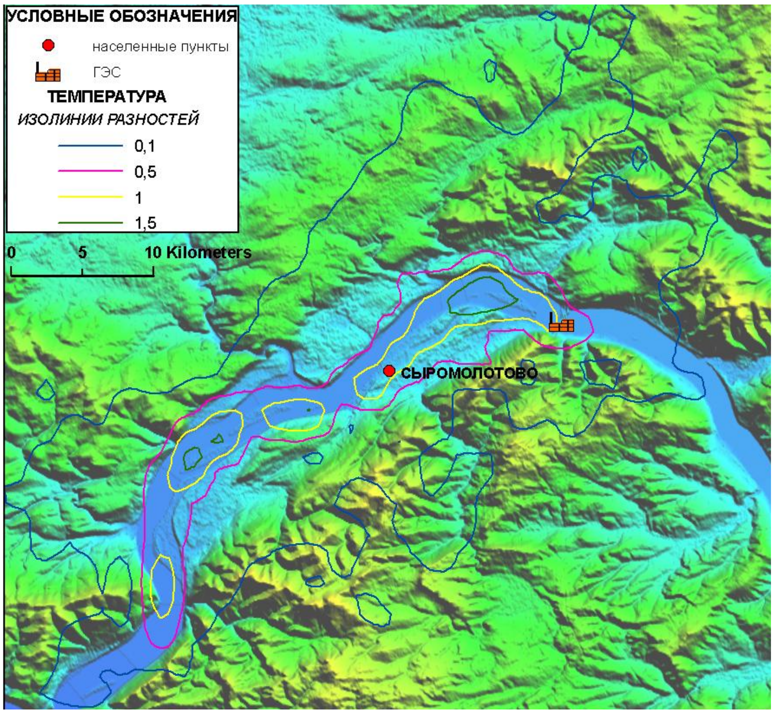


Fig.5.6.2. *Isolines of the temperature differences (deg. C) at the level of the surface layer in winter scenario /background flow is absent/.*

The significant changes in temperature and humidity fields spread to the distance of about 20 km from the unfrozen patch if the background flow is chosen as 2 m/s. The isoline of 1˚C –increase of temperature runs at the distance of 2-4 km from the patch in the lee side (Fig.5.6.4).

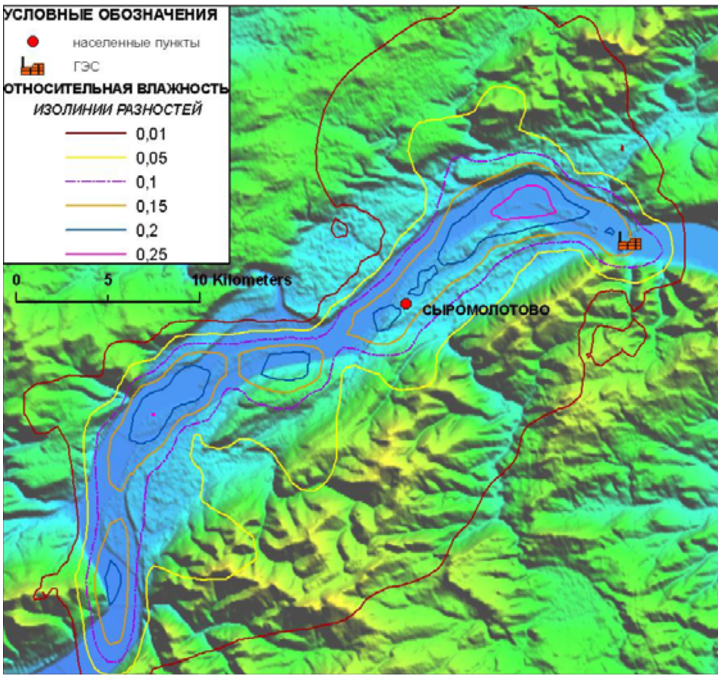


Fig.5.6.3. *The isolines of the relative humidity differences (10^{-2} %) at the height of the surface layer. The conditions of the calm background.*

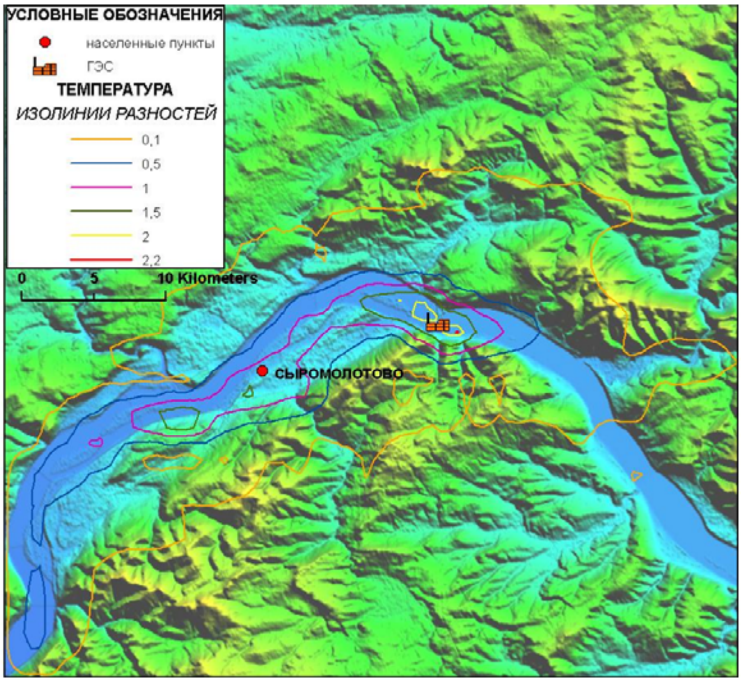


Fig.5.6.4. *The isolines of the temperature differences at the height of the surface layer. The western background flow of 2 m/s. winter season.*

In winter time the presence of even low background wind leads to the fact that the relative humidity on the lee side goes up. The isoline of 15% -increase of the relative humidity at the height of 60 m from the surface is situated at the distance of 1-2 km from the patch and moves away from the coast on the 3-4 km distance on the more gently sloping parts of the relief. The increase of relative humidity on 10% on the lee side of the patch extends on the 7-10 km along wind direction (Fig.5.6.5).

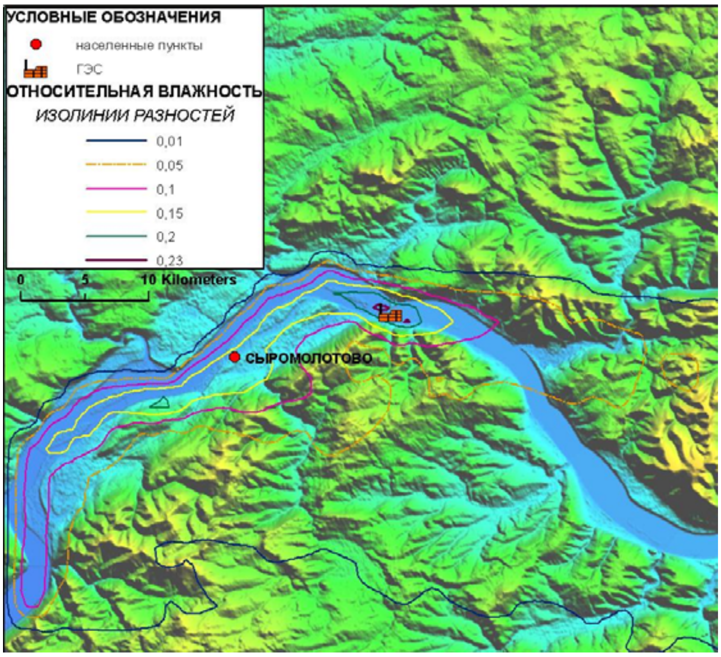


Fig.5.6.5. *The isolines of the relative humidity differences (10^{-2} %) at the height of the surface layer. The western background flow of 2 m/s. winter season.*

Summarizing one can conclude that the scenarios characterize the possible meso climate changes as insignificant for the territories distant from the coastline on about 10 and more km. But the direct influence of the reservoir and especially unfrozen patch will be significant in the nearest zone.

5.7. Localization of point emission source systems for advection-diffusion equation

We consider a localization algorithm for the system of point emission sources based on the point-wise measurement data. The algorithm is applied to the approximated localization problem which reduces to finding a metrical projection of the point in multidimensional space of measurement data onto the set of admissible cones. Each such cone is an abstract object defined by sources placed at the same location but having different emission rates. The cones are found with the help of adjoint problems formulated for the set of linear functionals each describing one measured datum. The metrical projection is found with the gradient-descent based optimization method.

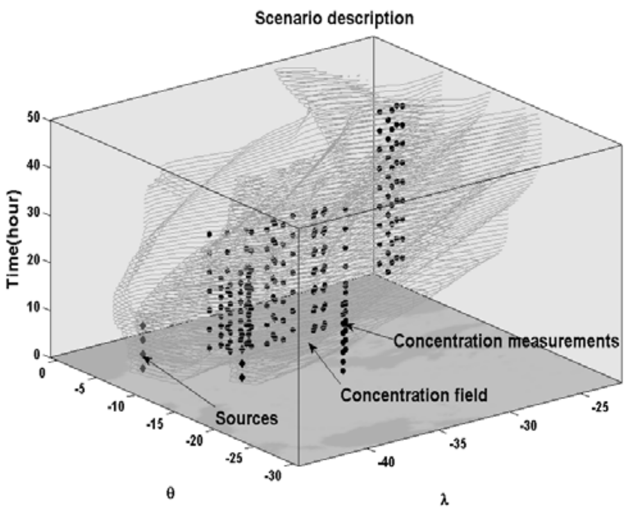


Fig. 5.7.1. *Scenario description*

Let there be a set of measurements of a substance concentration in the points of a spatial domain in the known time moments. This concentration field is supposed to be generated by an unknown system of point sources (Fig. 5.7.1). The problem is to find the locations of these sources. Here "point" sources are the sources of negligible area in comparison with the considered spatial scales (e.g. the area occupied by a power plant with respect to the grid domain cell size). The link between the substance concentration measurement data and emission source distribution is determined by means of adjoint equation approach applied to the atmospheric substance transport model (Marchuk, 1974, 1995). This approach is developed in the works (Pudikiewicz, 1998; Penenko and Baklanov, 2001; Penenko et al., 2002; Issartel, 2003). The authors look for a distributed source fitting the measurements with its subsequent interpretation in terms of point sources system. The interpretation task can be further simplified with the introduction of regularization that forces solution to have the smallest possible support (or vanish in the most part of the domain) as is done, for example, in (Krysta, 2007).
In this work we continue the study presented in (Penenko and Baklanov, 2001; Penenko, Baklanov, Tsvetova, 2002, Penenko A, 2008) by considering an alternative interpretation scheme of adjoint sensitivity functions. Our adjoint sensitivity functions interpretation scheme resembles, in some sense, the one considered in (El Badia, 2005; Hamdi, 2007; Agoshkov 2000). It interprets measurement data in terms of point source systems from the very beginning.

Localization problem statement

Given M known linear combinations

$$f_\mu = \sum_m \beta_{\mu m} \varphi(\lambda_{\mu m}, \theta_{\mu m}, \eta_{\mu m}, t_{\mu m}) \in \mathrm{R}_+$$

of values of the grid function $\varphi : \omega_T \to \mathrm{R}$ denoting an atmospheric substance concentration field in the $M(\mu)$ known points $p_{\mu m} := (\lambda_{\mu m}, \theta_{\mu m}, \eta_{\mu m}, t_{\mu m})$, $m \in M(\mu)$ of the grid domain ω_T with known weights $\beta_{\mu m}$. Here the grid domain ω_T is a discretization of the cylinder $\omega_T = \Omega_T^h = \Omega^h \times 0, T]^h$, where Ω is the rectangular domain in a three dimensional Euclidean space E^3, describing the part of the atmosphere. The measurement data can be represented as functionals

$$f_\mu = \left\langle \varphi, \sum_m \beta_{\mu m} \delta(. - p_{\mu m}) \right\rangle,$$

where $\delta(.-p_{\mu m})$ the Kroenecker delta-function is "situated" in the grid point $p_{\mu m} \in \omega_T$, and $\langle .,. \rangle$ is inner product in the space of grid functions.

Suppose the concentration field is the result of emissions from some sources $Q : \partial_{GRND}\omega_T \to \mathrm{Rp}$ placed at the Earth surface and is described by the operator equation

$$L\varphi = Q, \tag{5.7.1}$$

where $\partial_{GRND}\omega_T$ is the lower boundary of the grid domain, and $L : \omega_T \to \partial_{GRND}\omega_T$ is known linear operator. The right-hand side Q of the equation (1) has the structure

$$Q = \sum_{k=1}^{\Xi} q_k \delta(. - p_k), \quad q_k > 0, \Xi < \infty,$$

where the emission rates q_k and supports p_k are unknown and have to be found with the use of measured data f_μ.

Localizations in the measurement space

Let us denote any finite set $\bar{p} \subset \partial_{GRND}\omega_T$ by localization and describe how localization looks in the measurement space. To do this we introduce the operator of the direct problem $\widetilde{A}: Q \mapsto f$, which maps the source distribution function to the estimated "measurement result". The images of all the sources of all the capacities situated in points $\overline{p} := \{p_k, k = 1...\Xi\}$ of the spatial-temporal domain $\partial_{GRND}\omega_T$ constitute a cone

$$Cone(\overline{p}) := \{\overline{A}(\overline{p})q, q \geq 0\},$$

where

$$\overline{A}(\overline{p}) := [A(p_1) \quad \cdots \quad A(p_\Xi)], A(p) := \widetilde{A}(\delta(.-p)).$$

In order to find such a cone one can solve Ξ direct problems (1) and one has to repeatedly evaluate cones in the algorithm to be described. That is why we shall use the algorithm of $A(p)$ evaluation developed in (Marchuk, 1974) based on the adjoint problems. With this approach one only need to solve M adjoint problems to evaluate the cones.
Let linear operator $L^*: \omega_T \to \omega_T$, and linear function $\Psi: \omega_T \to \partial_{GRND}\omega_T$ be such that for any pair of grid functions φ and ψ

$$\langle L\varphi, \Psi(\psi)\rangle_{\partial_{GRND}\omega_T} = \langle \varphi, L^*\psi\rangle_{\omega_T}.$$

If φ solves the direct problem (1) corresponding to the sought Q and ψ_μ are the solutions of the adjoint equations

$$L^*\psi_\mu = \sum_m \beta_{\mu m}\delta(.-p_{\mu m}),\ \mu = 1,\ldots,M, \tag{5.7.2}$$

then

$$\langle Q, \Psi(\psi_\mu)\rangle = [\widetilde{A}(Q)]_\mu = \left\langle \sum_m \beta_{\mu m}\delta(.-p_{\mu m}), \varphi \right\rangle = f_\mu.$$

Weak statement of the localization problem

The formalism developed allows us to describe the fact that the measurements f register the system of sources located in $\overline{p}$ with the inclusion $f \in Cone(\overline{p})$. The problem of finding the cone can further be approximated by the problem of finding the cone (locally) minimizing the distance to the point f. With such a weakening, the problem boils down to the minimization problem

$$J(\overline{p}) = \min_{q_1>0,\ldots,q_\Xi>0} \left\| \overline{A}(\overline{p})q - f \right\|^2 \tag{5.7.3}$$

on the set of localizations.

Remark 1. Initial gridded setting is dictated by the fact that the solution of the direct and adjoint problems are obtained by the finite-difference algorithms. As the discrete solutions of the direct and adjoint problems converge to the corresponding continuous ones (except the source vicinities) with the mesh refinement, it is possible to extend the grid function $A(p)$ to the differentiable function on $\partial_{GRND}\Omega_T$ in order to use the smooth optimization methods.

To match the spatial-temporal scales in $\partial_{GRND}\Omega_T$ the metrics

$$\rho^2(p_1, p_2) = [p_2 - p_1]^* diag(L_\lambda^{-2}, L_\theta^{-2}, L_t^{-2})[p_2 - p_1]$$

should be introduced into $\partial_{GRND}\Omega_T$ where $p_i \in \partial_{GRND}\Omega_T \subset E^2 \times 0, T], i = 1,2,$ and L_λ, L_θ, L_t are the dimensions of the domain $\partial_{GRND}\Omega_T$.

Minimization of the objective functional on the set of localizations

Properties of the objective functional

The solution of localization problem is non unique. It follows from the antitonicity of the functional (3) with respect to inclusion: $\bar{p}_1 \subset \bar{p}_2 \Rightarrow J(\bar{p}_1) \geq J(\bar{p}_2)$.
To evaluate the functional (3) in general case, one should solve the constrained quadratic programming problem

$$q(\bar{p}) := \underset{q \geq 0}{\operatorname{argmin}} \left\| \bar{A}(\bar{p})q - f \right\|^2,$$

but the value can be found a bit easier in the special case:

- If $A(p_i)$ are orthogonal, then

$$J(\bar{p}) = \langle f, f \rangle - \sum_{k=1}^{\Xi} \langle A(p_k), f \rangle^2 / \langle A(p_k), A(p_k) \rangle.$$

- Let $A(p_i), i = 1 \ldots \Xi$ are linearly independent and

$$\bar{q} := \left[\bar{A}^*(\bar{p}) \bar{A}(\bar{p}) \right]^{-1} \bar{A}^*(\bar{p}) f \geq 0,$$

then $q(\bar{p}) = \bar{q}$.

One can always find a direction for the functional in which it decreases. Indeed, there is an $\alpha > 0$ such that

$$J(\bar{p} - \alpha \nabla_{\bar{p}} J(\bar{p}, q(\bar{p})), q(\bar{p} - \alpha \nabla J(\bar{p}, q(\bar{p})))) \leq J(\bar{p}, q(\bar{p})),$$

where

$$J(\bar{p}, q) := \left\| \bar{A}(\bar{p}) q - f \right\|^2,$$

$$\nabla_{\bar{p}} J(\bar{p}, q) = \left[\nabla_{p_1} J(\bar{p}, q) \quad \cdots \quad \nabla_{p_\Xi} J(\bar{p}, q) \right]^*,$$

$$\nabla_{p_k} J(\bar{p}, q) = 2 q_k \left\langle \nabla_\rho A(p_k), \bar{A}(\bar{p}) q - f \right\rangle$$

and ∇_ρ is a gradient operator with respect to metrics ρ.

Moreover in some cases one can uniquely identify the gradient. Let all $A(p_k)$ be linearly independent and $q(\bar{p}) > 0$, then the gradient with the respect to localization point p_k is

$$\nabla_{p_k} J(\bar{p}) = \nabla_{p_k} J(\bar{p}, q(\bar{p})). \tag{5.7.4}$$

Minimization algorithm based on gradient descent

Define a transition operator $S(\bar{p}) : \bar{p} \mapsto \bar{p}^\Xi$, where $\bar{p}^\Xi$ is calculated with gradient descent along the partial derivatives (5.7.4.) of the functional (5.7.3):

Algorithm 1. Let $\bar{p}^0 = \bar{p}$. By the recurrent evaluation

$$\bar{p}^l := \bar{p}^{l-1} - \alpha^l s^l, s^l := \left[0, \ldots, 0, \nabla_{p_l} J(\bar{p}^{l-1}), 0, \ldots, 0 \right]^*, l = 1, \ldots, \Xi,$$

where the descent parameter α^l is evaluated as the solution of the optimization problem

$$\alpha^l = \underset{\alpha > 0}{\operatorname{argmin}} \left[\min \left\{ J(\bar{p}^{l-1} - \alpha s^l), J(\bar{p}^{l-1}) \right\} \right], \tag{5.7.5}$$

with the method of golden section (e.g. see Vasiliev,1988).

Remark 2. It was practically discovered that the algorithm works slower if one takes the complete gradient $\nabla_{\bar{p}} J(\bar{p}, q(\bar{p}))$ instead of partial derivatives f^{l} as the descent direction. This can probably be explained by the fact that in iterations the different sources are situated on the different distances from their true locations that can lead to the ravine behavior of the functional in the vicinity of the current localization and in turn slowdown the descent.

Remark 3 . Relation (5) guarantees that the value of the functional $J(\bar{p})$ is non-increasing even if it has local minima .

As the solution is non-unique and the number of sources is unknown it is natural to start data fitting with one point source and gradually increase the number of points in localization till the functional (3) goes below the specified level. As the set of localizations of the cardinality $\Xi - 1$ is a subset of localizations of the cardinality Ξ, then the transition to a higher cardinality means a transition to the superset and the direction of such a transition corresponds to bifurcation of a localization point into two points moving in opposite directions. Based on these speculations the following algorithm can be introduced:

Algorithm 2. First point in localization is sought as a minimum of functional

$$J(\{p\}) = \langle f, f \rangle - \langle A(p), f \rangle^2 / \langle A(p), A(p) \rangle :$$

1. Given localization $\bar{p}^{\Xi-1} = \{p_1, ..., p_{\Xi-1}\}$ the following localizations are calculated

$$\bar{p}^{[i]} := \{p_1, \cdots, p_i - \delta p, p_i + \delta p, \cdots, p_{\Xi-1}\}, i = 1, \ldots, \Xi - 1,$$

where δp is small random perturbation with respect to the domain size. Optimization problem is solved to get the best extended localization:

$$\bar{p}^{\Xi} := \underset{\bar{p}^{[i]}}{\operatorname{argmin}} [J(S(\bar{p}))].$$

2. Stationary point of the transition operator is iteratively sought:

$$\bar{p}^{\Xi} := S^{\infty}(\bar{p}^{\Xi})$$

3. If $q_i(\bar{p}^{\Xi}) \le \varepsilon$, where ε is the specified small parameter, then the corresponding point p_i is removed from $\bar{p}^{\Xi}$.

4. Go to step 2.

Remark 4. In our numerical algorithm we use the normalized versions $A(p)/\|A(p)\|$ and $f/\|f\|$ instead of operator $A(p)$ and measurement data f correspondingly. This change is also dictated by our computational experience.

Localizing point emission sources in the Europe

Model of atmospheric advection-diffusion

Consider a domain

$$\Omega = \{(\lambda, \theta, \eta) \mid \lambda \in \lambda_{\min}, \lambda_{\max}], \theta \in \theta_{\min}, \theta_{\max}], \eta \in 0,1]\},$$

parameterized with coordinates (λ,θ,η), where $\left(\lambda,\frac{\pi}{2}-\theta\right)$ are spherical coordinates on the sphere of radius a (equal to the Earth radius) and η is a hybrid vertical coordinate with $\eta=1$ corresponding to the Earth surface and $\eta=0$ corresponding to the upper boundary of the atmosphere (we used coordinate system of HIRLAM model (Unden et al., 2002).
On the domain consider the advection-diffusion model

$$\frac{\partial\varphi}{\partial t}+\bar{u}\cdot grad\varphi-\frac{1}{m}div(mKgrad\varphi)=0,(x,t)\in\Omega_T \tag{5.7.6}$$

$$K\frac{\partial\varphi}{\partial n}-\bar{u}_n\varphi=0,\ x\in\partial\Omega_T/\partial\Omega_{TGRND}, \tag{5.7.7}$$

$$K\frac{\partial\varphi}{\partial n}-\bar{u}_n\varphi=Q,\ x\in\partial\Omega_{TGRND}, \tag{5.7.8}$$

$$\varphi|_{t=0}=0, \tag{5.7.9}$$

where

$$grad\varphi=\left[\frac{1}{a\cos\theta}\frac{\partial\varphi}{\partial\lambda}\quad\frac{1}{a}\frac{\partial\varphi}{\partial\theta}\quad\frac{\partial\varphi}{\partial\eta}\right]^*,$$

$$div(\Phi_x,\Phi_y,\Phi_z)^*=\frac{1}{a\cos\theta}\frac{\partial\Phi_x}{\partial\lambda}+\frac{1}{a\cos\theta}\frac{\partial(\cos(\theta)\Phi_y)}{\partial\theta}+\frac{\partial\Phi_z}{\partial\eta}, \tag{5.7.10}$$

$\partial\Omega_T$ is the boundary of the domain $\Omega_T=\Omega\times 0,T]$, $\partial\Omega_{TGRND}$ is the lower boundary of the domain Ω_T, $\bar{u}$ is the velocity vector, K is the diffusion tensor

$$K=diag\{K_x,K_y,K_z\},$$

$m=\frac{\partial p}{\partial\eta}>0$ where p is pressure. The latter obeys the continuity equation (Unden et al., 2002)

$$\frac{\partial m}{\partial t}+div(m\bar{u})=0, \tag{5.7.11}$$

which allows us to recast (5.7.6) as

$$\frac{\partial(m\varphi)}{\partial t}+div(\bar{u}m\varphi)-div(mKgrad\varphi)=0. \tag{5.7.12}$$

Domain Ω_T is approximated by the uniform grid domain ω_T with the mesh spacing $\Delta\lambda$, $\Delta\theta$, $\Delta\eta$, Δt and numbers of points $N\lambda$, $N\theta$, $N\eta$, Nt correspondingly.
Then the discretization is carried out for (5.7.6)-(5.7.9) considering (5.7.11) in order to fulfill balance relations and monotonicity of the resulting numerical scheme.
The coefficients are calculated with the use of given horizontal wind velocities (u,v), temperature T, surface-level pressure p_S, hybrid vertical coordinate system coefficients $H_1(\eta)$, $H_2(\eta)$ (Unden et al., 2002):

$$p(\lambda,\theta,\eta,t)=H_1(\eta)+H_2(\eta)p_s(\lambda,\theta,t),$$

$$m=\frac{\partial p}{\partial\eta}.$$

Vertical velocity $\dot{\eta}$ is calculated from the boundary value problem (Unden et al., 2002)

$$\dot{\eta}|_{\eta=0}=0,$$

$$\frac{\partial (m\dot{\eta})}{\partial \eta} = -\left(\frac{\partial m}{\partial t} + div_H(m(u,v))\right).$$

where div_H is the horizontal part of the div operator (5.7.10).
The horizontal diffusion coefficients are evaluated according to

$$K_x = K_y = K_h = K_{h0} + \frac{1}{2}\kappa^2 \Delta x \cdot \Delta y \sqrt{\left(\frac{\partial u}{\partial x} - \frac{\partial v}{\partial y}\right)^2 + \left(\frac{\partial v}{\partial x} - \frac{\partial u}{\partial y}\right)^2}$$

where $K_{h0} = 0.003\frac{\Delta x \cdot \Delta y}{\Delta t}$, $\kappa = 0.4$, $\frac{\partial}{\partial x} = \frac{1}{a\cos\theta}\frac{\partial}{\partial \lambda}, \frac{\partial}{\partial y} = \frac{1}{a}\frac{\partial}{\partial \theta}, \Delta x = a\cos\theta\Delta\lambda, \Delta y = a\Delta\theta.$
The vertical diffusion coefficient is calculated as

$$K_z = \left(-\frac{1}{m}\frac{q \cdot p}{R \cdot T}\right)^2 \begin{cases} K_{z0} + l_K^2\sqrt{U}\frac{R_{ic} - R_i}{R_{ic}}, R_i < R_{ic} \\ K_{z0}, R_i \ge R_{ic} \end{cases}$$

where

$$U = \left(\frac{\partial u}{\partial z}\right)^2 + \left(\frac{\partial v}{\partial z}\right)^2 + \varepsilon, \varepsilon = 1e-9,\ K_{z0} = 1, l_K = 40, R = 287,\ R_{ic} = 0.257 \cdot \left(-\Delta p\frac{R \cdot T}{g \cdot p}\right)^{0.175},$$

$$R_i = \frac{g}{\theta \cdot S}\frac{\partial \theta}{\partial z},\ \theta = T \cdot \left(\frac{p_s}{p}\right)^{0.288},\ \frac{\partial}{\partial z} = \left(-\frac{1}{m}\frac{g \cdot p}{R \cdot T}\right)\frac{\partial}{\partial \eta}.$$

Numerical experiments

In the numerical experiments the spatial domain represents the European atmosphere. Meteorological data to calculate model coefficients of (5.7.6)-(5.7.9) are provided by the Danish Meteorological Institute (Sass,1994) and correspond to the period from 23 October 1995 to 27 October 1995 (86 hours). As the prototype of the measurement system we used the subset of all the measurements taken in the experiment etex1_v1.1.960505 (Archer et al.1996), which constituted 168 measurement stations.
The emphasis in our work was made on the development of the computational algorithm for the inverse source localization problem. That is why we present the results of purely computational experiment where we excluded all the uncertainties introduced by the imperfections of our substance transport model. In our experiment the scales are kept real and the measurement data has been fabricated with the solution of the direct problem (5.7.6)-(5.7.9).
The grid domain parameters are 100*100*40 points with the mesh spacing (0.2288°,0.3128°,1/40).
To check whether the algorithm is robust, some results are presented for the different random data perturbations δf. The perturbed data f^δ has been calculated according to the standard formula

$$f^\delta = f + NoiseLevel \cdot \|f\|\frac{w}{\|w\|},$$

where w is a normally distributed random vector.
In order to measure the value of each source found with respect to the complete localization, we introduced the following system of weights. Let $\overline{p} = \{p_1, \ldots, p_\Xi\}$ be localization. The weight w_i of $p_i \in \overline{p}$ is calculated as

$$w_i = \frac{\left\| \overline{A}(\overline{p} \setminus \{p_i\}) q(\overline{p} \setminus \{p_i\}) - \overline{A}(\overline{p}) q(\overline{p}) \right\|}{\left\| \overline{A}(\overline{p}) q(\overline{p}) \right\|}. \tag{5.7.13}$$

To exclude the noise components of the obtained solutions we dropped the sources with

$$w_i < \max(NoiseLevel, 0.01).$$

Scenario 1. Let there be two sources emitting a substance for 4 hours after the beginning of the experiment. On the 20th hour of the computational experiment the concentrations are measured by 168 measurement stations used in ETEX experiment. Measurements are evaluated according to the formula

$$f_\mu = \varphi(\lambda_\mu, \theta_\mu, \eta_\mu, t_\mu),$$

where φ is the solution of the direct problem. The data are passed to the source localization algorithm. In Figs 5.7.2-5.7.3 the final results are presented for the different random data perturbations δf .

Scenario 2. The sources locations are the same but the measurement system was taken according to ETEX experiment:

$$f_\mu = \frac{1}{n} \sum_{l=1}^{n} \varphi(\lambda_\mu, \theta_\mu, \eta_\mu, t_\mu + \Delta t \cdot (l-1)), \tag{5.7.14}$$

where $n = 3hours / \Delta t$. Measurements are taken by the complete ETEX measurement system within the intervals $[22hours, 24hours]$ and $[25hours, 27hours]$ according to (5.7.14). Results are presented in Figs. 5.7.4- 5.7.5.

Scenario 3. In this experiment we have changed the exact system of sources to one used in ETEX experiment (single source working with constant emission rate for 10 hours after the start of the experiment). The results are presented in Figs. 5.7.6- 5.7.7.

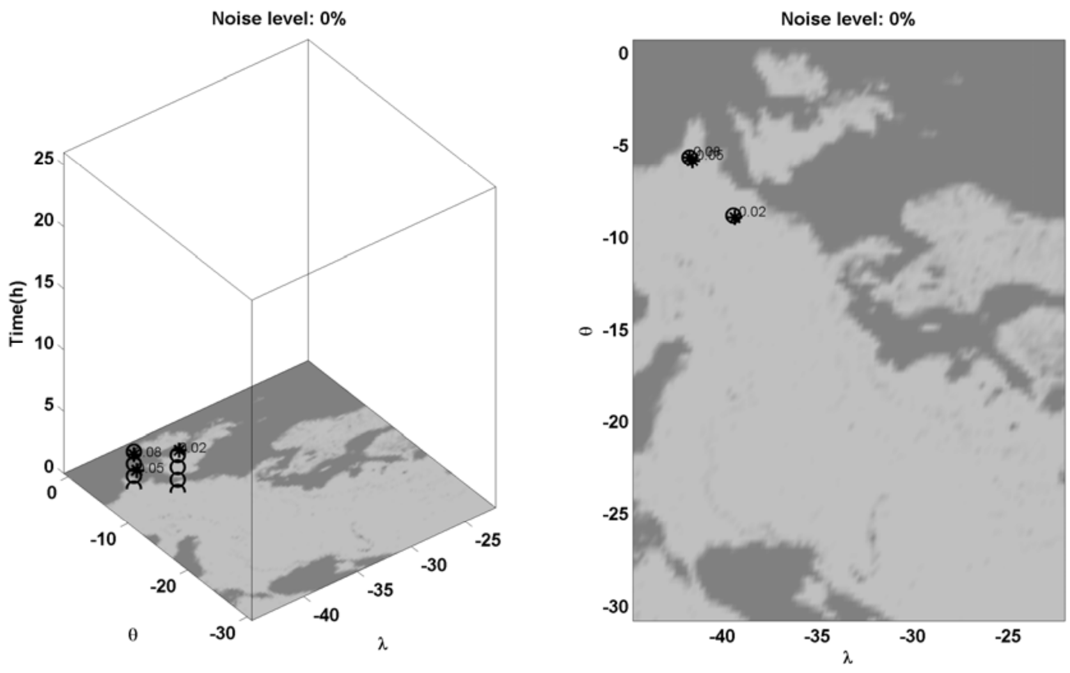


***Figure 5.7.2**: The results of reconstruction for Scenario 1. Asterisks show the reconstructed localization. Circles give the exact localization. Values near sources are their weights (5.7.13).*

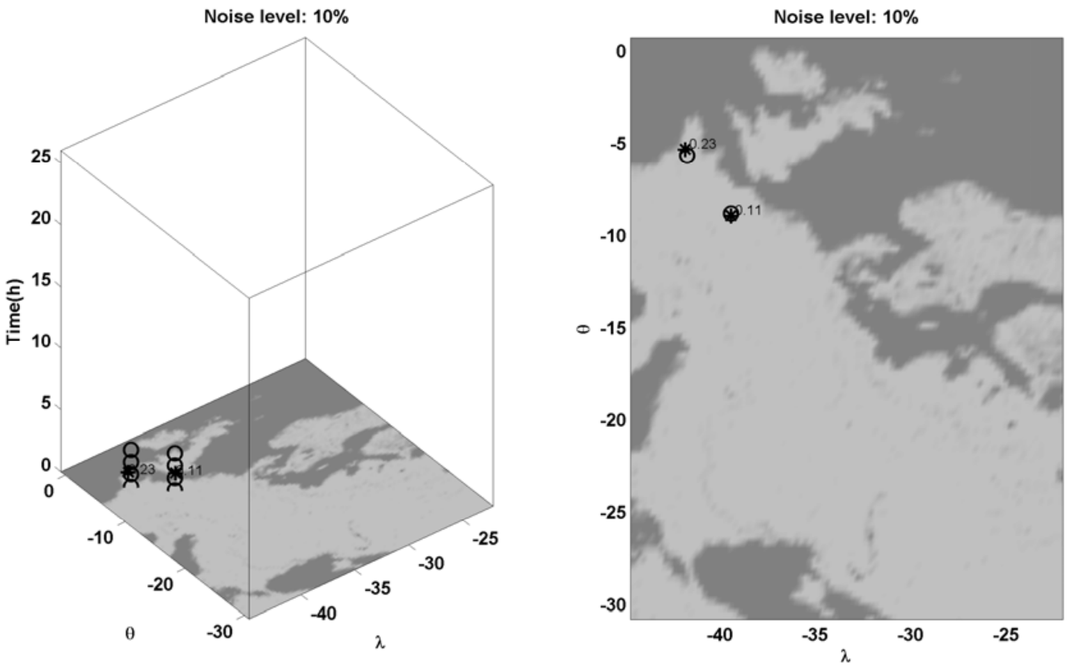


Fig. 5.7.3. *The same as in Fig.5.7.2 but for the noise level of 10%*

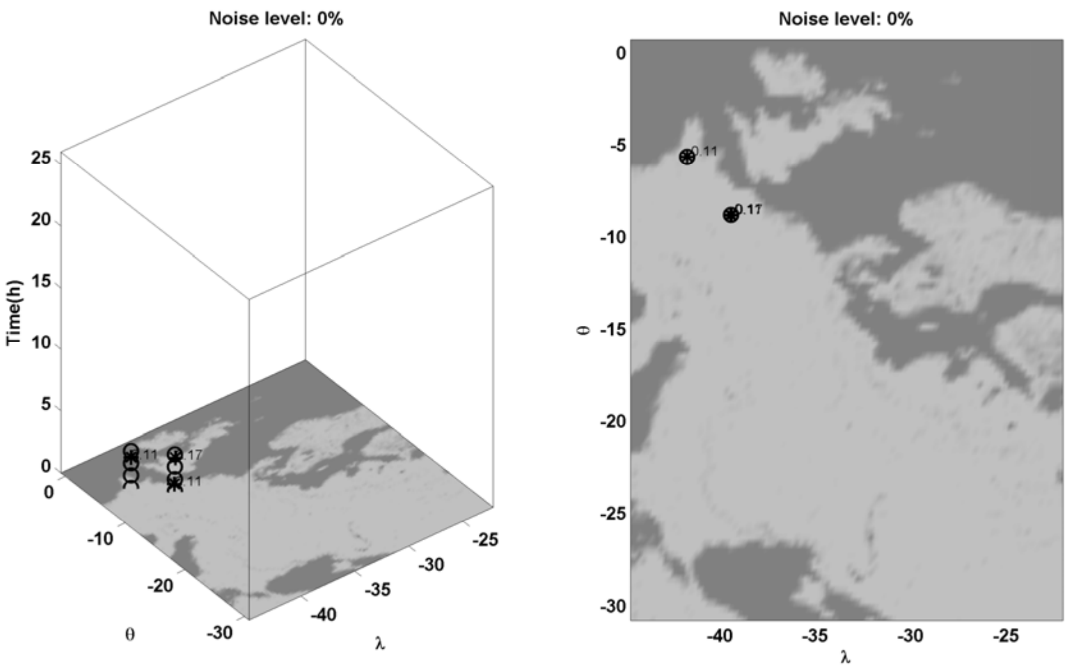


Fig. 5.7.4. *The results of reconstruction for Scenario 2. Asterisks show the reconstructed localization. Circles give the exact localization. Values near sources are their weights (5.7.13).*

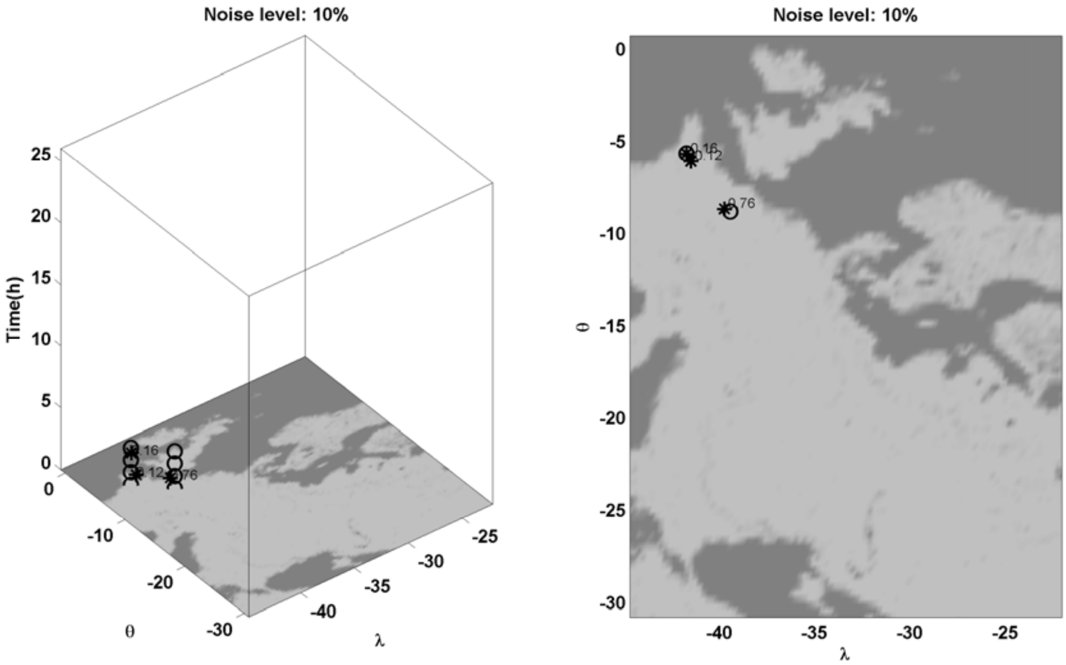


Fig. 5.7.5: *The same as in Fig.5.7.4 but for the noise level of 10%*

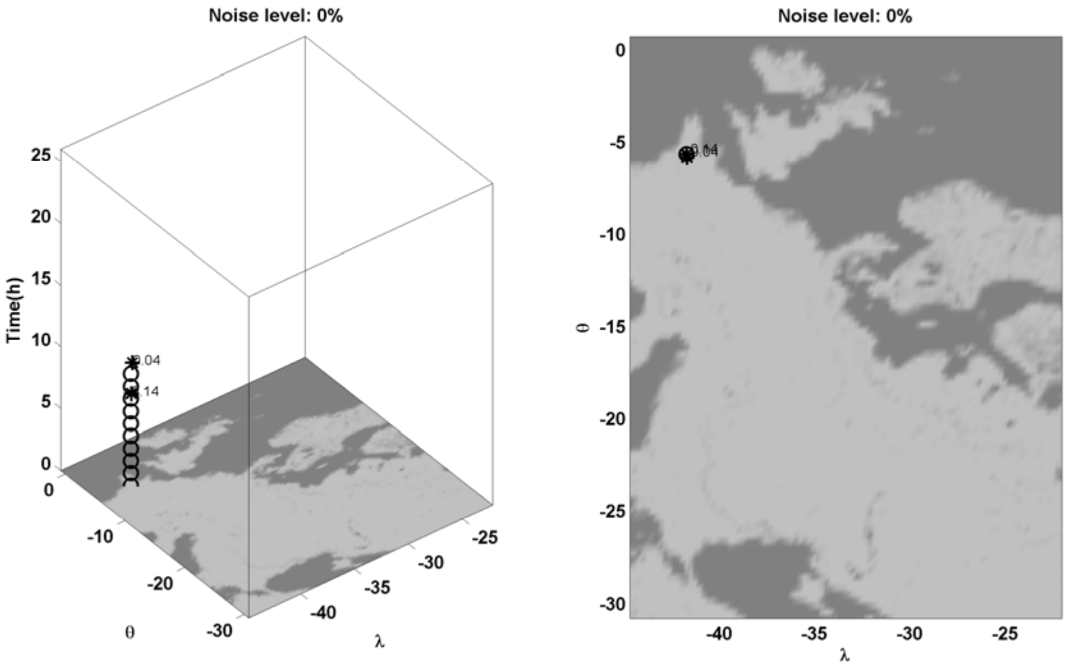


Fig. 5.7.6. *The results of reconstruction for Scenario 3. Asterisks show the reconstructed localization. Circles give the exact localization. Values near sources are their weights (5.7.13).*

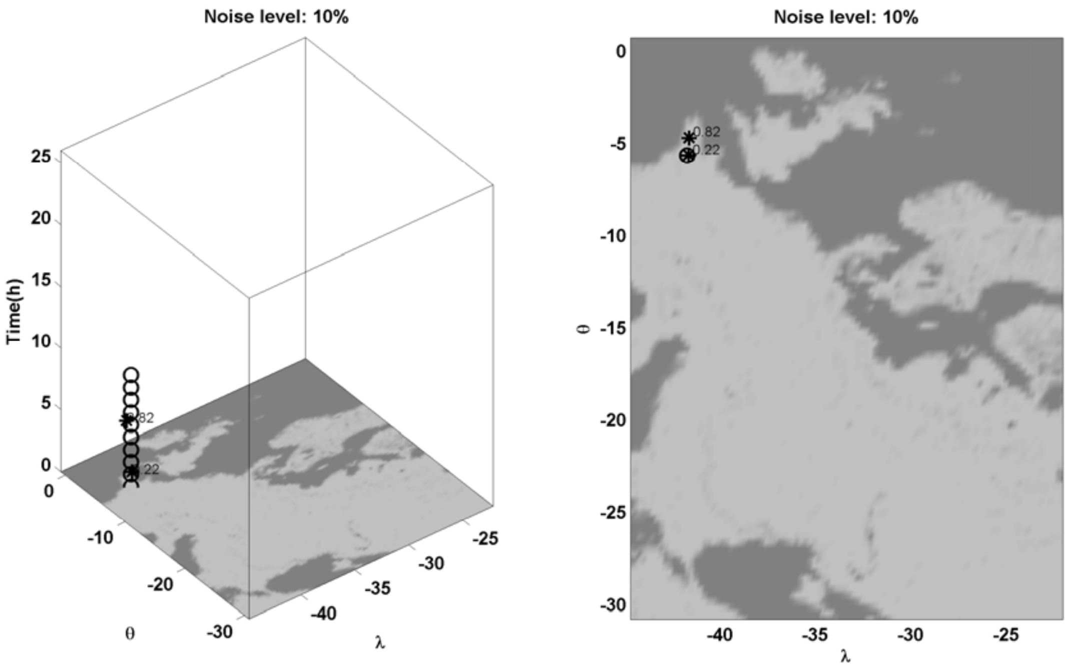


Fig. 5.7.7. *The same as in Fig.5.7.6 but for the noise level of 10%*

Point source localization problem was recast to the problem of finding a cone containing the point. The set of admissible cones was constructed with the solution of adjoint problems for the advection-diffusion equation. A gradient-descent based algorithm has been used to solve the problem in the weak optimization statement. The results of numerical experiments show that in the case of exact data our algorithm provides good results and in the perturbed data case the figures show a robustness of the algorithm with respect to noise.

The results obtained give us optimistic vistas for the considered approach to the source localization problem. At the next stage along with the further development of the source localization algorithm itself, we also consider utilization of a better substance transport model and investigation of adaptive observations targeting algorithms to minimize the errors in reconstruction results using the adjoint modeling at minimal additional cost.

Conclusions and Recommendations from Focus Topic: Atmospheric Pollution and Risks

State of the art of research in Siberia

The tendencies in environmental modelling in Siberia can be shortly characterized in the following way. There are some leading groups of environmental modelers in Novosibirsk, Tomsk, Irkutsk, Krasnoyarsk, Tumen, Barnaul, Kemerovo, Yakutsk, Ulan-Ude, Chita, Omsk, and Khanti-Mansiisk. These groups belong mainly to the institutes of the Siberian Branch of the Russian Academy of Sciences.

There are three tendencies in the usage of modelling tools in these groups:

- using simplified regulatory models (Gaussian type, one/two dimensions, a few parameters, etc.), (about 50-60 %)
- adopting well-known internet-available models, like MM5, WRF, HYSPLIT, etc. (20-30 %, increasing)
- developing original comprehensive models of different complexity from local to global

scales (10-15%, decreasing).

A comparative analysis of about 30 numerical models for environmental studies was made on the materials of 10 conferences of different level. Some concrete recommendations on numerical realization of the models were made on the basis of own partners' theoretical findings. And some applications of the approaches developed by partners are given and discussed in the reports.

As for risk assessment, there are some approaches known in the world practice. The first one is direct approach in which the forward problem is used to obtain the solution. The second one uses the inverse methods based on the solution of adjoint problems and sensitivity analysis. The mixed strategies are also applied. The partners develop all these approaches.

It should be noted that there is some specificity is environmental RTD activity in Russia and consequently in Siberia. There is some sort of "specialization of labor" between science and practice. As a rule, the routine data of observations on weather, atmosphere-water-soil quality, sources of emission, etc. are gathered and concentrated in the hydrometeorological and resource state services whereas the theoretical studies are the prerogatives of the Academy of sciences. There is some experience when co-operation gave positive results in the solution of environmental problems of Siberian Federal District. One of the recent events was the Workshop on "Integrated system for the meteorological elements and air quality forecasting and assessment of emission in the atmosphere of megalopolis, transport nodal points and other objects of infrastructure" (October, 2008). The specialists from academician institutes (INM, ICMMG, IMCES), from Siberian Research Institute of Hydrometeorology of Roshyromet and the end-users' representative from the Novosibirsk region administration (Vice-governor G.A.Sapojhnikov) discussed the current state of studies and future plans of innovations to the environmental policy in Novosibirsk region.

Recommendations on future research

The specific character of Siberian region consists in the fact that it is necessary to study the processes on the vast territories under their insufficient lighting by the data needed for the model initialization and scenario construction. Taking into account these circumstances, we would recommend the following:

- To solve environmental problems on a modern level, we suggest elaborating the concept of environmental modelling based on application of variational approach and solution of inverse problems as fully as possible. With the help of variational principles one can generate almost all necessary computational algorithms, sensitivity theory methods for models and functionals, control theory methods and methods of direct and inverse modelling.
- To assimilate observational data, the models of observations (the models presenting the results of measurement in terms of the state functions) should be consistently designed with the models of processes.
- Till now, the problem of sources revealing and identifying is a weak spot in the algorithm of risk control. As the problem is nonlinear and high dimensioned, a methodology guarantying the unique solution (if it exists) in the case of many sources, is not designed yet. This part of work needs to be theoretically studied further.
- Specific models for emergency situations, when adequate quantitative assessments and optimal solutions are necessary, should be developed. The most important point here is an immediate assessment of situation when the input data are incomplete.
- Scenario approach is an important part of environmental modelling. To construct long-term forecasts and risk estimates one needs an appropriate methodology which is able to obtain the results taking the possible climate changes into account. Here the advanced approach is the use of informative bases and the methods of orthogonal decomposition of multi-dimensional phase spaces that describe the different characteristics of the phenomena under study.
- Since the methodology of analysis and prognosis is based on the joint use of models and data, it is naturally to make efforts to include as many as possible of admissible types of observa-

tional data while solving environmental problems. The synergy effects of mutual co-ordination are pronounced in the construction of the thematic data bases and data processing, in the development of the methodology of data assimilation and targeting observational programs. Such co-operation should be continued in future.

It is necessary to underline that the risk assessment problems as well as the problems of estimation of changes in climate-ecology system belong to the problems of the higher system level than the ordinary problems of transport and transformation of pollutants. The former are essentially dependent on the results of the latter. Therefore we need to improve the basic models and algorithms to cope with the following tasks:

• To assess uncertainty in the models and input data for increasing the intervals of predictability under the incomplete information supply;
• To enhance the skill of atmospheric chemistry models and models of the system “gases + aerosols”. To these aims one needs to improve the algorithms for stiff systems in forward and adjoint modes, to use adaptive monotonic algorithms, and to overcome the problems of non-consistency such as monotonizators, self-limiting diffusion for divers components, etc.
• To develop a targeting data assimilation including chemical data assimilation for reconstruction of the current state and emission assessment;
• To construct the cost-effective methods for solving the optimal problems for design of sustainable strategy of environment development;
• To develop the technology for analysis and synthesis of the scenarios and their results.

Some modifications are necessary to the numerical models, designed on the traditional approaches of forward modelling and developed earlier by different scientific teams, to be used in the context of inverse modelling. Their immediate use for the goals of adjoint sensitivity analysis and risk assessment, inverse modelling and data assimilation gives rise to definite difficulties due to the inconsistency of numerical models in forward and adjoint modes. One of the constructive ways to overcome such problems is the immersion of the forward model codes to the specific version of a variational principle, in which the appropriate procedures of generalized differentiation of the functionals and operators with respect to the state functions and parameters provide obtaining the exact gradients of evaluated cost functionals.

Almost all above mentioned problems are intensively attacked in the world and the partners of the project and the other colleagues from Siberian teams are taking part in the theoretical and applied studies.

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