Interdisciplinary investigations of transport and transformation of admixtures in the atmosphere: tentative results and prospects

V.V. Penenko* and M.V. Panchenko

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

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We describe here the main principles of work organization in a interdisciplinary team of researchers from several institutes of Siberian Branch of the Russian Academy of Sciences (SB RAS) as applied to realization of one of two subprojects of the integration grant (IG) SB RAS–97 No. 30. The project is devoted to investigation of the processes of transport and transformation of admixtures in the atmosphere of Siberia. More than 50 scientists took part in this work. The presented material shows that already at this stage of realization of the subproject we succeeded in accomplishing, say, the most complicated organizational task, namely, joining the researchers (chemists, physicists, mathematicians, meteorologists, and geographers) for team-work on the urgent interdisciplinary problem. Besides, we have provided the monitoring regime of atmospheric observations, and even for this short period of observations we have obtained the data, which will give an essential progress in comprehension of the nature of physical and chemical processes in the atmosphere and in improvement of numerical models for description and prediction of these processes.

Introduction

The main approaches to the study of natural processes proceeding under the effect of natural and anthropogenic factors in order to solve problems of ecology, environmental protection, and climate are now formulated. They are based on combination of fundamental laboratory investigations, network and field observations within regular monitoring systems and specialized observational experiments, analysis of data, and mathematical simulation.

These principles formed the basis for the work of an interdisciplinary team of researchers from institutes of Siberian Branch of the Russian Academy of Sciences (SB RAS) on one of two subprojects of the integration grant (IG) SB RAS–97 No. 30. This project was devoted to investigating and simulating processes of transport and transformation of admixtures in the atmosphere of Siberia. More than 50 scientists took part in this project. Main organizations taking part the project and leaders of the corresponding sections are, respectively, Institute of Computational Mathematics and Mathematical Geophysics (Novosibirsk), Dr. V.V. Penenko; Institute of Chemical Kinetics and Combustion (Novosibirsk), Dr. G.I. Skubnevskaya and A.N. Akilov; Institute of Thermal Physics (Novosibirsk), Dr. A.P. Burdukov; Institute of Atmospheric Optics (Tomsk), Dr. M.V. Panchenko; L.A. Melent'ev Institute of Power Systems (Irkutsk), Dr. B.M. Kaganovich; Limnological Institute (Irkutsk), Dr. T.V. Khodzher; Institute of Solar-Terrestrial Physics (Irkutsk), Dr. V.V. Koshelev; Omsk Affiliate of the Institute of Mathematics, Dr. V.A. Shaptsev.

Due to joint efforts, a large cycle of research on the basic aspects of the problem has been carried out. Below we discuss the tentative results of this work and formulate our plans for the future.

1. Models of transport and transformation of admixtures in the atmosphere

The conceptual grounds and principles of the set of basic multifunctional models for diagnostic and prognostic purposes have been developed. The set is an open developed system in its physical content and the class of solved problems, in the functional structure of models, in the methods of implementation, and in comprehension. A pilot version of the set of models has been implemented, and the cycle of research into the processes of admixture transport on various spatiotemporal scales has been carried out.

Goals and problems:

– Estimation of ecological prospect for different variants of anthropogenic impact;

– Ecological prediction and design;

– Monitoring and estimation of efficiency of nature-protection measures;

– Estimation of characteristic scales of interactions in the climatic system.

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Main characteristics of the models, their structure, and functional content:

– systems of basic equations of atmospheric transport and transformation of multicomponent admixtures from natural and anthropogenic sources;

– related problems for a certain set of functionals;

– algorithms for calculating the sensitivity of models to variations of parameters and external actions;

– algorithms for direct and inverse simulation.

The basic versions of the models are implemented in the local, mesoregional, hemispheric, and global scales. The versions of mesoscale models adapted to the conditions of Novosibirsk, Tomsk, Omsk, and Irkutsk are also available.

Simulation scenarios are organized based on methodology of direct and inverse simulation and the joint use of models and observation data.

Models of admixture transport on the local scale and mesoscale operate together with models of hydrothermodynamics of the atmosphere that provide calculation of atmospheric circulation characteristics from the available actual information in the regime of assimilation and prediction with the required resolution.

To organize simulation scenarios on the regional and global scales, a new class of models is developed for reproducing atmospheric circulation using databases of actual information (so-called models of information type). To provide the validity of estimates in these models, retrospective actual information on the atmospheric circulation by the Reanalysis NCEP/NCAR (USA) data is used. A specialized program package has been developed for operation with this information. It includes algorithms of data assimilation and hydrodynamic interpolation with the use of basic models of atmospheric hydrothermodynamics. This software provides reconstruction of the fields of meteorological elements with the spatiotemporal resolution required for admixture transport models in the regimes of direct and inverse simulation. With such an approach, the question on predictability of atmospheric circulation does not arise. Now we have an access to the daily information (two observations a day) over 38 years (1961–1998) that allows us to solve many research problems.

2. System for simulation of the processes of chemical transformation of admixtures in the atmosphere

A highly efficient system for simulation of kinetic processes of chemical transformation of pollutants emitted by both natural and anthropogenic sources in the atmosphere of an industrial region has been developed. The system allows fast formation of numerical models of chemical kinetics by the given schemes of transformation mechanisms and calculation of the time behavior of the corresponding processes. In its structure, the system is a component of the set of models developed to solve nature-protection problems of prediction of chemical conditions in emergencies. The system is intended for the use in two aspects: (1) in autonomous, spatially point-like regime for studying time behavior of processes and (2) as a part of the set of transport models described in Section 1, as a set of point-like kinetics models in the regime of splitting within four-dimensional spatiotemporal models.

To provide the efficiency and high operating speed of the simulation system, two new basic elements have been developed. The first one is a unit for preparing "chemical" models of transformation of substances. It is based on a preprocessor of kinetic schemes that allows automatic construction, in the interactive regime, of the system of differential equations of chemical kinetics using descriptions of transformation mechanisms as a set of reaction equations presented in the traditional chemical form. This is the most technically complicated and labor-consuming stage in developing models, and it is completely automated with the use of the preprocessor. The automaton system is convenient for research tasks, since during the work one often needs to reconstruct reaction schemes and change the description of transformation mechanisms. All these operations are performed in the interactive regime.

The second key element is the algorithm for solution of kinetic equations in the spatially point-like regime. For a basic version of the algorithm, stable implicit schemes of the second order of accuracy are constructed. Since the problems of chemical transformation are nonlinear, the algorithm for their solution is organized so that the procedure of recursive increase of the accuracy of approximation by nonlinearity is initiated if necessary. Parameters for quantization of the kinetic equations are selected with regard for the characteristic lifetime of substances taking part in reactions.

It should be noted that from the computational viewpoint the described class of problems requires large computer resources both in the number of operations and in the computer memory (ROM and RAM). To find a compromise, problems of atmospheric chemistry are parallelized using the splitting method into, on the one hand, the set of advection-diffusion problems for simulating the transport of individual substances in space and, on the other hand, the set of point-like problems, in which at the every time step the processes of transformation of all substances at every point of the spatial grid are formally independent of the systems of equations at other points. To increase the efficiency of simulation, parallel versions of the earlier developed algorithms are under development at the Institute of Computational Mathematics and Mathematical Geophysics. In the future they will be implemented at the supercomputer center of SB RAS.

The "chemical" block of admixture transformation, which is developed at the Institute of Chemical Kinetics and Combustion and the Institute of Power Systems, employs the international database of chemical gas-phase reactions compiled at the USA National Institute for Standards and Technologies. It includes more than ten thousand chemical reactions allowing chemical parameters to be varied widely in the automatic regime. Due to this, modeling pollutant transformations in the atmosphere, we succeeded to obtain fundamental results more closely adapted to actual conditions.

The procedure of joining the kinetic models with the database was worked out using photochemical oxidation of acetaldehyde as an example. Acetaldehyde is the most representative element of the class of carbonyls in the atmosphere. We chose elementary stages causing formation of ecological carcinogens: formaldehyde, methanol, as well as carbon oxide and dioxide. It was shown that at different combinations of the initial emissions of aldehyde with nitrogen oxides the toxicants listed above are formed in different relations. Besides, the ozone concentration in the surface atmospheric layer changes markedly on local scales.

The block of preparation of the initial chemical information and kinetic models have been numerically implemented at the Institute of Power Systems. Specialized software has been developed to automatize construction of kinetic schemes. This software allows coordinated operation of the preprocessor of these schemes and the database of kinetic information. Using the point-like photochemical model of the atmosphere of mid-latitudes that was developed at the Institute of Power Systems, the sensitivity of the concentrations of some secondary pollutants to emissions of typical gaseous waste of power engineering (unsaturated hydrocarbons and nitrogen oxides) has been studied. The strongly nonlinear character of this dependence has been revealed, and it has been shown that there exist conditions under which the effect of hypersensitization arises.

3. System for estimation of atmospheric quality and prediction of consequences of emergency and ecologically unfavorable situations in industrial regions

The prediction system under development is based on the set of models of hydrothermodynamics and admixture transport in the atmosphere of urban and industrial regions. The system is designed to solve specific environmental problems connected with estimation of the atmospheric quality and ecological safety for people and natural systems. For starting preparation of the set, the efficient method of calculating the initial fields from minimal actual information has been developed. This problem becomes especially urgent now because of the high risk of technogenic emergencies (practically in all branches of economical activity) and war conflicts.

Models of this class are characterized by high spatiotemporal resolution. They require voluminous actual information on the current state of the climatic system for provision of computations. Therefore, these models usually operate well for estimation of situations in the scenario regime, since this regime does not require very fast preparation of a solution and there is considerable freedom in the choice of input data.

Several versions of models for solution of nature-protection problems of large cities are presented in the project.

The system for estimation of the ecological prospect within the scenario approach for emergency and normal situations is under development at the Institute of Computational Mathematics and Mathematical Geophysics.

The main problem for operation in emergency and extreme cases for a specific region is efficient and adequate initialization of models and issue of a prognosis. The factor of time is decisive in this case. We have developed a version of the mesoscale numerical model for solution of such problems. In this version, models are initialized and prediction is given based on limited actual information.

The system of prediction and model initialization by the proposed method was tested using particular problems for the Novosibirsk and Tomsk regions. The spreading of admixtures at the emergency at the Tomsk Radiochemical Plant in April 1993 is very interesting example, since for this period we have observation data. Comparative analysis of calculated and measured fields of radioactive pollution has demonstrated their close agreement in configuration and intensity of the zone of increased pollution. This agreement indicates good potentialities of the set of models as far as concerned reconstruction and prediction of actual situations and efficient initialization of models by limited actual information.

A modification of the model of atmospheric dynamics and admixture transport has also been developed to study and predict atmospheric pollution in Omsk. It has formed a basis for a performed series of numerical experiments on estimation of the atmospheric quality in Omsk for some specific situations. Dialog algorithms for determination of parameters of sources from measured admixture concentrations have been developed and implemented.

4. Models for solution of related problems of ecology and climate

The concepts, basic principles, and structure of the set of models of the system “atmosphere of industrial region” have been formulated. This set of models is intended for solution of related problems of ecology and climate. It includes both sources of pollution and other anthropogenic effects, such as, for example, changes of the characteristics of the Earth’s surface at large areas, heat release and moisture emissions in large volumes, etc. Such impact on the climatic system gives rise to specific atmospheric processes. They, in turn, give rise to ecologically unfavorable and even catastrophic situations. We have developed the theory and methods for investigating the sensitivity of the climatic system of industrial regions to variations of natural and anthropogenic factors. This allows revealing of the effect of relatively weak factors on the general characteristics of the climatic system.

In this class of problems, absolute values of anthropogenic impact are relatively small as compared to the main factors determining the behavior of the climatic system and the quality of the atmosphere. The problem is to recognize and quantitatively estimate the effect of these small factors and order them by the relative contribution to variability of observed characteristics. To solve this problem, we have constructed the algorithms for realization of the relations of the sensitivity theory and calculation of the sensitivity functions of functionals determining the general characteristics of the behavior of the models under study.

Estimation of the sensitivity of atmospheric radiative conditions to changes of the concentrations of optically active admixtures should be set off. The estimates show that the effect of gaseous pollutants and aerosols on thermodynamics of the atmosphere of industrial regions can be significant. This effect manifests itself differently in different situations.

The sensitivity relations allows us to estimate variations of corresponding functionals directly from variations of the parameters of pollution sources without detailed calculation of radiative conditions of the polluted atmosphere. This approach gives a new solution to many problems, since calculation of the radiative conditions of the atmosphere is a very labor-consuming process, especially as climatic investigations suppose long-term measurements.

5. Development of techniques for measurement and experimental estimation of parameters of pollution sources

The techniques for direct measurement of the parameters of pollution sources and estimation of emission factors have been developed.

In the system of fast prediction in normal and, especially, extraordinary situations, information on the actual emissions of pollutants is very important. From this point of view, methods for measuring the parameters of pollution sources, pollutant concentrations, and fields of meteorological elements fit organically into the system of provision of numerical models.

The techniques for direct measurements of source parameters have been developed at the Institute of Thermal Physics. Thermal power stations No. 1, No. 2, and No. 4 situated in environs of Novosibirsk Akademgorodok were chosen as objects of study (choice was conditioned by their proximity to Akademgorodok and limited funding available). Pollutant concentrations were measured with a PEM–2M gas analyzer. This analyzer is a computer system that operates in the regime of long unattended measurements, stores measurement results, and transmits them to a personal computer through the corresponding interface. The gas analyzer is equipped with a heated sampler with a temperature sensor and sample preparation unit. The concentrations of following gases were measured: CO_2, CO, NO, NO_2, SO_2, and O_2.

Since the device is capable of storing measurement results and transmitting them to a PC, having installed such devices at every station and joined them into a network, we can obtain the data on actual sources of pollution in real-time. Such information is necessary for real-time monitoring and prediction of the atmospheric quality. Therefore, implementation of the developed measurement technology is very urgent and can be recommended to official monitoring systems.

Specialists from the Institute of Power Systems have determined and refined some ecological indices of boiler-houses of medium and low power, as well as smoke furnaces. The results of these works give important initial information for prediction of the processes of pollution of Siberian cities. A series of comparative experiments on burning of Siberian coal and firewood has been successfully completed. For studied fuels, specific emissions of sulfur, nitrogen, and carbon oxides, solid particles, soot, and polycyclic aromatic compounds have been calculated. The factors determining variations of emission indices for these substances have been revealed. Continuous monitoring of CO in the atmosphere of Irkutsk has been carried out. Limiting seasonal variations of gas pollution of the atmosphere with the products of partial combustion of fuels have been determined. It has been confirmed that smoke furnaces contribute to carbon monoxide pollution of the atmosphere of old Siberian cities.

6. Experimental studies of transport and spatiotemporal scales of variability of pollutant content in the atmosphere of Siberia

The Institute of Atmospheric Optics, Institute of Chemical Kinetics and Combustion, Limnological Institute, and Institute of Solar-Terrestrial Physics were responsible for the experimental part of the project. They dealt with development of the concept of purposeful monitoring, measurement techniques, and techniques for processing of experimental results in order to judge peculiarities of spreading of aerosol and gaseous pollutants in the Siberian atmosphere and prospects of their usage for diagnostic and prognostic studies. The concept of the purposeful monitoring consists, in essence, in combination of a small number of stationary monitoring stations with wide use of mobile laboratories equipped with multifunctional measuring equipment and based on ground and air vehicles. In accordance with this concept, the monitoring system must actively interact with mathematical models in the feedforward and feedback modes: planning of observations, estimation of comprehension of the monitoring systems, diagnostics of quality of models, data assimilation, etc.

The main experimental goal of this project was organization of observations in a region for studying the processes determining formation of gas and aerosol composition of the atmosphere, revealing a role of natural and anthropogenic components, and studying characteristic sources and directions of admixture transport. This is a necessary stage of estimating the interactions of the type "source – sensor" and "sensor – – source" with the use of mathematical simulation.

The key point of an observational experiment in a region is obtaining the information on the complete, if possible, set of atmospheric parameters, their annual and seasonal variability as applied to geophysical conditions of the Siberian region, determining the characteristics of spatiotemporal variability of aerosol and gaseous components of the atmosphere, and describing their relations with external geophysical factors.

Siberia, which combines wide non-urbanized territories and large industrial centers, is still poorly investigated in this respect. Creation of a wide network of stationary monitoring stations is a problem that cannot be solved today because of economic and technological reasons. A way out of this situation is combination of a small number of posts operating in the nearly monitoring regime with organization of large-scale complex experiments involving the maximum number of systems providing measurement of most climatically and ecologically significant atmospheric parameters.

Besides, it is necessary to use a limited number of mobile laboratories on ground and air carriers operating in expeditionary conditions.

The use of results obtained at space stations extends essentially the capabilities of analysis of regional data. For this purpose, the project involved Centers of Space Monitoring at the Institute of Solar-Terrestrial Physics and Institute of Atmospheric Optics, which dealt with reception and fast processing of satellite information for the Siberian territory.

Such organization of studies at a wide territory provides obtaining data for well-founded testing and improving the prognostic models.

In the process of realization of the project at the Siberian territory, we succeeded to organize synchronous long-term observations in three geographic zones (Tomsk, Novosibirsk, and Irkutsk), in sites subject to anthropogenic impact and being under "background" conditions.

In Tomsk, Novosibirsk, and Irkutsk, surface measurements are carried in the nearly monitoring regime at automated stations disposed at the Akademgorodok territory. In each of these regions, observations are complemented with regular expeditionary cycles carried out in regions far removed from large industrial centers. In Tomsk, it is the proving ground of the Institute of Atmospheric Optics on the River Ob; in Irkutsk, it is the station of the Limnological Institute in the Listvyanka village on shore of Lake Baikal; in Novosibirsk, it is the station of the Institute of Chemical Kinetics and Combustion in the Chik village. Thanks to cooperation with the National Institute for Environmental Studies (Japan), in last two years we succeeded in carrying out monthly sensing of the atmosphere with the airborne laboratory of the Institute of Atmospheric Optics. Thus, we have passed to the qualitatively new level of the possibilities in interpretation of the whole collection of data.

The significance of observations under background conditions should be emphasized. In our region, Sayanskaya Solar Observatory (Mondy village) plays the part of the basic background station for studying admixture transport in the lower atmosphere of South-Eastern Asia. The station Mondy (51°10′ N, 109°20′ E) is the astronomical observatory on the mountain top (2000 m) of the ridge Khamar-Daban which is more than 300 km far from industrial centers of the Baikal region. Now there are strong grounds for believing that the station Mondy will be included into the international network of stations for monitoring of acid fallouts in the Eastern-Asian region (EANET) that will start in 2000.

Space information can be accessed on the server of the Center of Space Monitoring: http://ckm.iszf.irk.ru. This server also presents the results on detection of forest fires (four times a day) in the form of electronic maps. Besides, it allows one to view photos of the cloud cover over the Siberian territory in statics and dynamics.

Conclusions and prospects

As is seen from the presented material, already at this stage of the project we succeeded in solving, say, the most complicated organizational problem, namely: in joining the efforts of many researchers (chemists, physicists, mathematicians, meteorologists, and geographers) for solution of the urgent multidisciplinary problem. Besides, we have provided the monitoring regime of observations needed for atmospheric problems and have obtained the data, which will provide a progress in comprehension of the nature of physical and chemical processes in the atmosphere, as well as in improvement of numerical models for description and prediction of these processes.

One of the applied results obtained in the project is development of the technique (set of models and monitoring methodology) for real-time estimation of scales of interactions in the climatic system, in particular, regions of danger arising because of ecological catastrophes. Besides, the developed techniques allow us to estimate the efficiency of monitoring systems and the variability of comprehension areas of these systems in actual atmospheric situations.

More than 90 papers became the results of these investigations. The list of the papers is too long to be presented here, but one can find it in the report by the project IG SB RAS No. 30 "*Investigation and simulation of global and regional climate changes, transformation and transport of admixtures in the atmosphere of Siberia*," Novosibirsk, 1999.

As far as concerned our plans for the future, it should be noted that, in spite of the significant progress achieved in the world at the current state of science and technology, many questions concerning the atmosphere and biosphere are still open.

These questions mostly deal with physical-chemical, ecological, and climatic aspects of aerosols and minor gaseous constituents of the atmosphere acting as pollutants. These pollutants affect directly and indirectly the state of the biosphere and ecosystems, human health, quality of the atmosphere and water, as well as behavior of the climatic system. Let us analyze the evolution of climatic-ecological ideology. At the early stages, the attention of researchers was focused at CO_2 as a main factor in anthropogenic stimulation of climatic changes. Further, the importance of such chemically and optically active gases as methane, carbon monoxide, halocarbons, and ozone has been revealed. Some of these substances are produced in the biosphere. Variations of their concentrations on the regional and global scales are caused by human activity. They are so-called greenhouse gases contributing to climate warming.

Then it was found that aerosols also affect the global climate. For example, particles of sulfate produced by burning coals scatter a significant part of incoming solar radiation thus favoring cooling of industrially loaded regions. Therefore, studies of chemical and microphysical processes affecting formation and life cycle of such aerosols are of great interest. Since aerosol particles can serve as condensation nuclei at formation of clouds, aerosols of anthropogenic origin are capable of indirectly affecting the climate via changes of optical properties of clouds: optical depth and albedo.

There exist aerosols whose interaction with radiation has a complex character. For example, mineral particles can scatter and absorb ultraviolet, visible, and infrared radiation. This leads to either cooling or heating of the climatic system under certain hydrometeorological conditions. For example, soot of black coals has a tendency to absorb a part of solar and reflected radiation, what induces heating of the atmosphere.

Interaction of dust particles with other atmospheric aerosols and clouds can affect their properties. Interaction processes control heterogeneous chemical reactions and can form multicomponent aerosols. However, the relative role of these processes is still unclear. It should be kept in mind that the lifetime of mineral aerosols in the atmosphere is relatively short; it lasts about a week. Therefore, their effect is of regional scale and, hence, their ecological consequences can manifest themselves in the first turn. Aerosols affect not only climate. They play an important part in chemistry of the stratosphere and troposphere via many heterogeneous reactions and affect significantly the intensity of photolytic processes (change of visibility, damage of vegetation, and damage to human health). The problems of formation of the life cycle, transport, and possible action of biologically active aerosols, as well as related problems of ecological safety acquire now a particular urgency.

Thus, the world community has yet to solve many problems concerning the environment and climate. Our interdisciplinary team has obtained significant results on many of the problems mentioned above. Therefore, we intend to continue our investigations assuming that only joint efforts in interdisciplinary teams provide the basis for successful advance.

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