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Abstract: The limitations of the widespread methods of air pollution level estimation allow producing quite rough air quality estimations for the areas not covered by observation stations. Application of the computational models to this purpose requires usage of the meteorological observations, atmospheric emissions of industrial enterprises, measurements of the concentration of the atmospheric pollutants as well as the numerical modelling of the gaseous substance transformation and transport processes. High accuracy of estimation and forecast of air quality for such models are achieved with the use of information on pollutant emission from sources within the city and distribution of the meteorological parameters obtained with the use of model of atmospheric boundary layer. In this report the results of the work devoted to creation of the web-system (http://air.risks.scert.ru/tomsk-mkg/) for effective air chemical composition assessment and forecast in the conditions of industrial city area and its suburbia are presented. Tomsk city air pollution estimation data obtained as an output of the pollution transport mathematical model has been employed as a research basis for selected periods from 2000 to 2006. The air quality model is based on prognostic transport equations taking into account chemical reactions of air pollutants on the basis of reduced model of chemical reactions. Dynamic and thermal characteristics of the atmospheric boundary layer (ABL) are calculated on the basis of simplified model of urban ABL. Working version of the dedicated web-application has been created based on the web-portal ATMOS engine. At present it allows to estimate such characteristics as average monthly and seasonal pollutions for chosen time interval of the day along with their yearly dynamics as well as daily dynamics for various pollutants such as sulphur dioxide, nitric oxide, carbon monoxide, dust, etc. The web-system being considered could be used for long duration ecological risks assessment as well as for calculation of pollution scenarios resulted from different technological breakdown events for various meteorological conditions.

Keywords: Air pollution; Ecological monitoring; Web applications; Meteorology.

1. INTRODUCTION

Atmospheric boundary layer processes have an essential impact on the biosphere and human activity [Oke, 1987]. Even minor changes in moisture exchange and radiation balance between the Earth surface and atmosphere, chemical composition of the air and other characteristics may have serious consequences for environment. For this reason one of the key tasks in the area of environment preservation at present is modelling of atmospheric processes and creation of applied Internet-accessible information-computational systems aiming at monitoring and forecast of ecological and meteorological conditions of atmospheric boundary layer. In particular, this task becomes very important in the current period of rapid development of industry, power engineering and road network that causes permanent atmospheric air deterioration due to increase of the number of factors affecting its chemical and aerosol composition. During the past decades simulation models have been widely used for scenario computations designed for clarifying specific features of pollution propagation over chosen area under various meteorological conditions. Scenario analysis is performed to study the contribution of separate emission sources into general air pollution, as well as to estimate effects of possible emergency situations at extra-hazardous objects, such as nuclear power-stations, chemicals plants, etc. Simulation models are also included in on-line information systems for air quality monitoring and forecast. Such systems provide real-time detailed information on distribution of air pollution concentration over the urban territory, with the stationary observation data being used as initial and boundary conditions as well as for validation of calculation results.

It should be noted that analysis of the air pollution state can not be completed without taking into account the contribution of secondary emission products, i.e., resultants of chemical and photochemical reactions between constituents of anthropogenic emissions and atmosphere gases [Moussiopoulos et al., 1995]. Many of such compounds are highly toxic; they form so-called urban photochemical smog, which lowers the visibility and affects detrimentally human beings, animals and plants. At present many models are designed to estimate concentrations of secondary pollutants with a precision depending in many respects on the number of constituents being considered and connecting equations varying from tens to few hundreds for different procedures.

2. MODEL DESCRIPTION

Pollution transport mathematical model represents the model of turbulent diffusion, including the transport equations with the description of advection, turbulent diffusion and chemical reactions, which is applied to calculate the air pollutant concentrations taking into account the chemical changes [Belikov et al., 2005]:

$$\frac{\partial C_i}{\partial t}+\frac{\partial UC_i}{\partial x}+\frac{\partial VC_i}{\partial y}+\frac{\partial W_c C_i}{\partial z}=-\frac{\partial}{\partial x}\langle c_i u\rangle-\frac{\partial}{\partial y}\langle c_i v\rangle-\frac{\partial}{\partial z}\langle c_i w_c\rangle+S_i+R_i;\;\; i=1,..,n_s \qquad (1)$$

Here $C_i(t,x,y,z)$, $c_i(t,x,y,z)$ are pulsating and averaged constituents of i-components concentration of impurity respectively; u,v and U,V are pulsating and averaged horizontal components of wind speed respectively; w_c, W_c are pulsating and averaged vertical components of impurity speed; S_i represents emissions of i-component of impurity in the atmosphere; R_i describes generation and transformation of substance during chemical reactions; n_s is a number of chemical impurity components considering in the chosen scheme of chemical reactions.

Original expressions for turbulent fluxes $\langle c_i u\rangle \langle c_i v\rangle \langle c_i w_c\rangle$ are used in the given work [Belikov, 2006]:

$$-\langle c_i u\rangle=\frac{\tau}{C_{1\theta}}\left(\left(1-C_{2\theta}\right)\langle c_i w\rangle\frac{\partial U}{\partial z}+\langle u_j u\rangle\frac{\partial C_i}{\partial x_j}\right); \qquad (2)$$

$$-\langle c_i v\rangle=\frac{\tau}{C_{1\theta}}\left(\left(1-C_{2\theta}\right)\langle c_i w\rangle\frac{\partial V}{\partial z}+\langle u_j v\rangle\frac{\partial C_i}{\partial x_j}\right); \qquad (3)$$

$$-\langle c_i w_c \rangle = \frac{\tau}{C_{1\theta} + D_{1C} F}\left(-\left(1 - C_{3\theta}\right) \frac{g}{\Theta} \langle c_i \theta \rangle + \langle u_j w_c \rangle \frac{\partial C_i}{\partial x_j} \right). \quad (4)$$

Here $u_j = \left(u, v, w_c\right)$, F is the function defining the surface influence on the turbulent flow structure; $c_x = 5.0$, $C_{1\theta} = 3.0$, $C_{2\theta} = 0.346$, $C_{3\theta} = 0.333$, $D_{1C} = 0.806$ are empirical constants, $\tau = l / C_D \sqrt{k}$ is the time scale of turbulent pulsations, g is the gravity acceleration, θ, Θ are pulsating and averaged components of potential temperature. Repetitive index j means summation.

To calculate the unknown correlation of pulsations of temperature and concentration $\langle c\theta \rangle$ included in equation (4), the following differential equation is used:

$$\frac{\partial \langle c_i \theta \rangle}{\partial t} + U_j \frac{\partial}{\partial x_j} \langle c_i \theta \rangle = -\langle c_i w_c \rangle \frac{\partial \Theta}{\partial z} - \langle \theta u_j \rangle \frac{\partial C_i}{\partial x_j} + \frac{\partial}{\partial x_j} \left(\alpha \frac{k}{\varepsilon} \langle u_k u_j \rangle \frac{\partial \langle c_i \theta \rangle}{\partial x_j} \right) - \frac{2}{\tau \cdot c_x} \langle c_i \theta \rangle; \quad (5)$$

$$i = 1,..,n_s; \;\; j = 1,..,3; \;\; k = 1,..,3.$$

Expressions (2)-(4) have the form of the Boussines gradient ratio: $\langle c u_i \rangle = -K_{ij} \dfrac{\partial C}{\partial x_j}$.

Turbulent flows of heat and impulse, included into the derived expressions (2)-(4) are defined using the algebraic ratios presented in [Starchenko, 2000].

3. PROBLEM FORMULATION

Mainly this work is devoted to creation of the web-system (http://air.risks.scert.ru/tomsk-mkg/) for effective air chemical composition assessment and analysis in the conditions of industrial city area and its suburbia. At present detailed pollutant concentration fields were obtained as an output of the pollution transport mathematical model described earlier for selected periods from 2000 to 2006. Dynamic and thermal characteristics of the atmospheric boundary layer are calculated on the basis of simplified mesoscale model of urban ABL developed at the Tomsk State University and Institute of Atmospheric Optics RAS.

The problem was solved numerically in the investigated domain that covers an urbanized territory with numerous high-rise point sources, as well as linear, point and area emission sources situated on the underlying surface. Predictions were performed with the use of finite volume method and new explicit-implicit calculation scheme of solving three-dimensional prognostic transport equations at Skif-Cyberia multiprocessor systems of Tomsk State University.

Here the dataset obtained as an output of pollution transport and transformation mathematical model was put onto the powerful server and provided with basic software toolset accessible via unified web-interface for data processing and visualization and subsequent analysis. Web-portal ATMOS software [Gordov et al., 2006], specially designed for rapid development of scientific applications, has been used as a base for web-system development. Graphic user interface of the system is planned to realize using DHTML technology for it allows to provide more friendly user interface than standard HTML [Okladnikov and Titov, 2006]. PHP scripting language is used for implementation of relevant program modules within the framework of ATMOS web-portal. The work is devoted to the practical realization of the working version of the dedicated web-application for effective air quality assessment of the city area [Gordov et al., 2007].

4. SYSTEM FUNCTIONAL DESCRIPTION

The system being developed comprises three following parts:

- Generated by the model [Belikov et al., 2005] data archives containing detailed fields of the pollutant concentrations for selected for each season periods in 2000-2006 interval
- Graphic user interface
- A set of PHP-scenarios to perform data processing and conversion with the following visualization

It should be noted that raw data archives obtained as a result of numerical modelling are incompatible with the data used by the system for a number of technical reasons, so that first they were structured and converted into the standard binary format used by GrADS software package for the following online visualization.

Graphic user interface is developed based on the web-portal ATMOS engine and represents dynamic HTML form to enter calculation and visualization parameters (Figure 1).

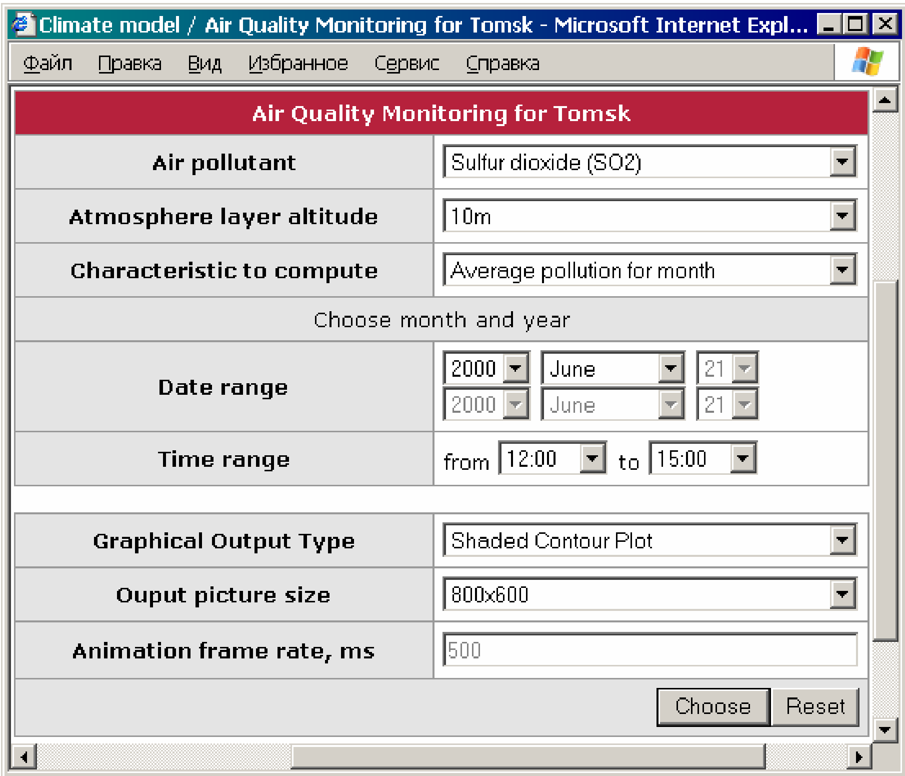

Figure 1. Dynamic HTML form for entering calculation parameters

The form allows setting the following parameters:

- "Air pollutant" with such values as airborne particulate matter, sulfur dioxide, nitrogen dioxide, carbon oxide and ozone)
- "Atmospheric layer altitude" ranging from 10 to180 meters
- "Characteristic to compute". At present it is possible to calculate such characteristics as average pollution for month and season for chosen time of the day and their dynamics within the selected time interval as well as hourly dynamics for the selected day

- Date range, time range, graphical output type and picture size. There's also a possibility to choose animation frame rate to see dynamics of the pollutant concentration.

"Date range" fields allow to set the time interval of interest. It should be noted that contents of the fields is generated dynamically according to the model data currently available for processing. It is an important issue from the point of view of effective access to relevant information because model computational process is very heavyweight so that output data can be received in relatively small blocks. It is also possible to set "Graphical output type" and animation frame rate. After the form is filled in and calculations are carried out web-application will render the results on the screen.

5. CURRENT RESULTS

Below several examples demonstrating present capabilities of the web-system are to be found. Figure 2 shows average nitrogen dioxide pollution of the Tomsk city area for September, 2006 from 6.00 pm till 9.00 pm.

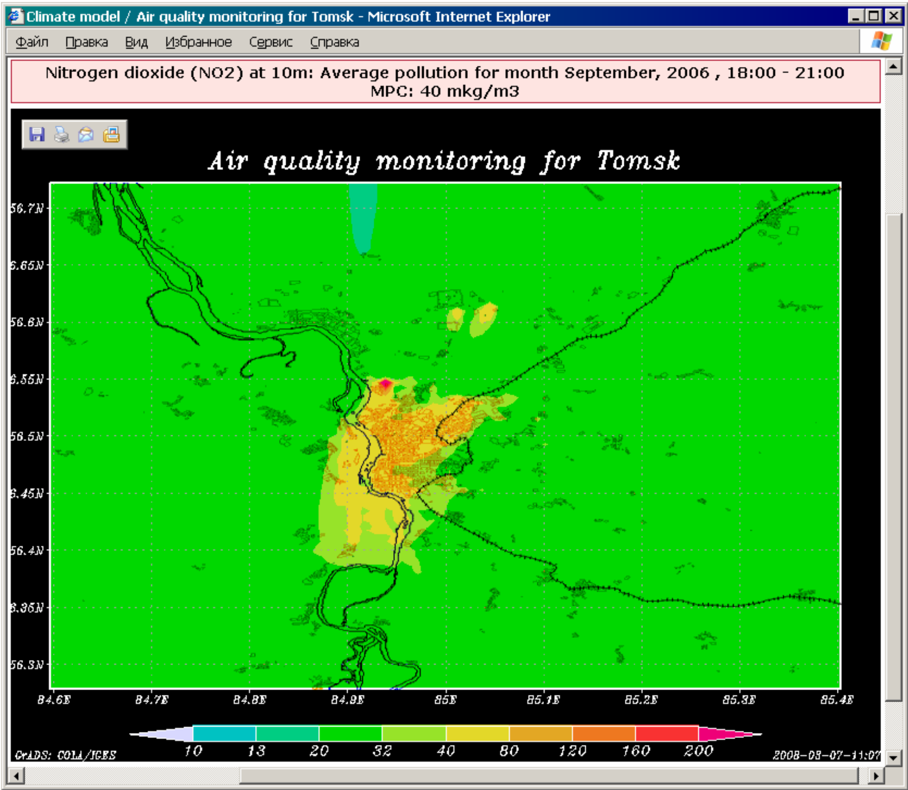

Figure 2. Average NO_2 pollution at 10m for September, 2006, 18.00 – 19.00.

It should be noted that the scale displayed on the graphics generated by the system is normalized according to the corresponding maximum permissible concentration value residing in the middle of the scale that makes the picture easy for interpretation.

The functional capability of the system of calculating monthly and seasonal averages for a number of years and representing them in animation mode would be useful for analysing pollutant concentration dynamics. Table 1 that follows below shows an example of visualization of average seasonal SO_2 pollution for 6 years.

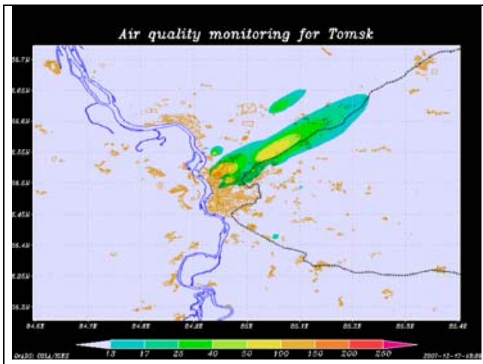

Figure 3. Winter, 2001

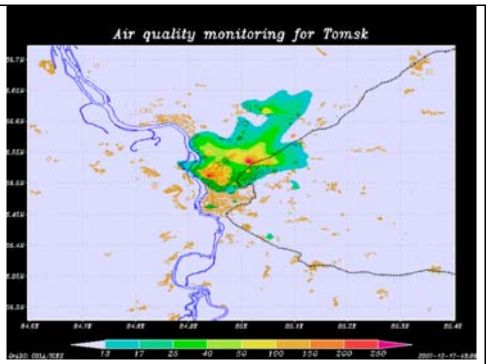

Figure 4. Winter, 2002

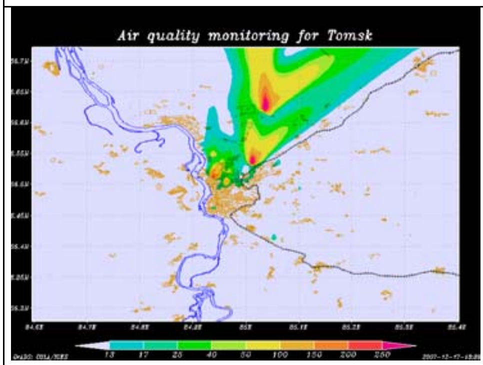

Figure 5. Winter, 2003

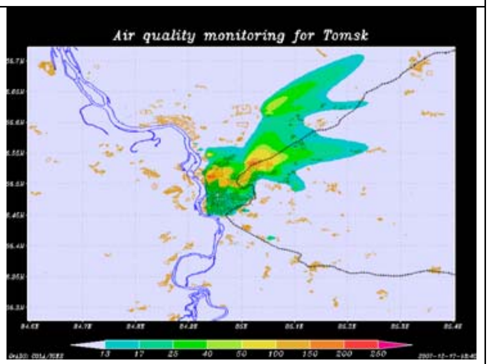

Figure 6. Winter, 2004

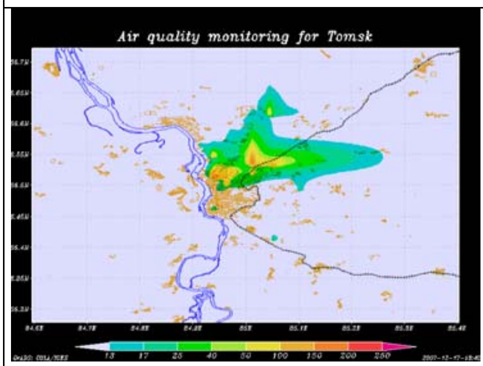

Figure 7. Winter, 2005

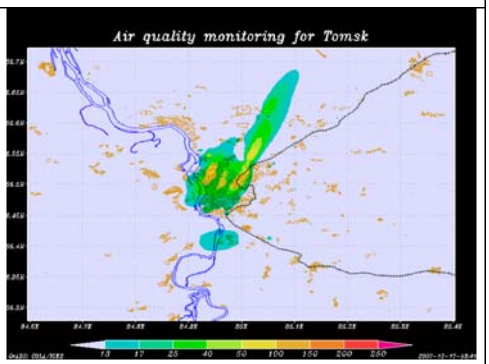

Figure 8. Winter, 2006

Table 1. Dynamics of the average SO2 pollution for winter season at 10m, 12.00 – 15.00.

6. CONCLUSION

The system is aimed at regional ecologists and decision makers and provides them with images of pollutant concentrations fields at different altitudes for the industrial city area. It might be used to determine characteristics of pollution distribution above the territory and their dynamics under different weather conditions, to estimate input of selected pollution sources (industry enterprises, transport, etc.) into pollution fields, as well as to estimate consequences of possible accidents leading to additional pollutants blowouts. Also it might be used to understand degree of anthropogenic influence on regional environment and climate. It should be added that the system has generic character and being provided with characteristics of industrial and transport pollution sources, local meteorology data, surface properties and generated by the pollution transport and transformation mathematical model datasets it can be easily adjusted for conditions of an arbitrary city.

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