Application of the WRF-CHEM mesoscale model to investigation of vertical and horizontal structures of low atmosphere in Tatarstan

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Received February 26, 2007

Results on the study of spatio-temporal variations of the real nonstationary atmosphere are presented. Outcomes of numerical modeling of 3D spatial inhomogeneities of meteoparameters, some impurities, and their dynamics are considered. The analysis is made for the East-European region in view of real underlying surface inhomogeneities and unsteady weather conditions using the up-to-date model of atmospheric chemistry and impurities transfer WRF-CHEM. The comparison of the computed time series with experimental data has shown a good agreement. Local vertical and horizontal structures of the gained perturbations are studied, including the case of the concentration of atmospheric impurities.

Introduction

At present, the study of the local structure of meteorological regime of the boundary layer and air pollution combines math modeling and empiric-statistical approach. Pollutant propagation models are intensively developed for solving the problems of environmental monitoring.[1–3] To use mesoscale models in forecasting the fields of meteoparameters and atmospheric pollutants, the assignment to a particular geographic region and a choice of different schemes of parameterization of atmospheric processes are necessary. Verification of chosen numerical model's parameters is possible in conditions of regular survey of meteoparameters and atmospheric pollutant concentrations.

We have the unique data in hand of every-minute monitoring of meteoparameters and pollutants from 1996 to 2006 at the network of spatially spaced stations in the East-European region of Russia (Aznakaevo town (54.85°N, 53.1°E); five stations spaced by 1 to 6 km in Al'met'evsk town (54.9°N, 52.3°E); Zelenodol'sk town (55.85°N, 48.5°E); Kazan city (55.8°N, 49.1°E); two longitudinally 2.5-km-spaced stations in Minnibaevo town (54.8°N, 52.2°E). Analysis of these data reveals complexity and irregularity of actual atmospheric processes, resulting in temporal and spatial variations of most parameters, including concentrations of trace gases and aerosol.[4,5]

To study peculiarities of these variations, their formation and propagation, to detect the wave and macroturbulent components, their anisotropic dependence on the relief, it is important to obtain an adequate model of inhomogeneities, allowing the study of both horizontal and vertical perturbations in a specific geographical region and in local climatic conditions.

Origination of an instantaneous 3D picture of lower atmosphere and its dynamics directly from the hydrodynamics equation and real initial and boundary conditions seems to be the most adequate and informative approach to study the variations. Though, this approach requires complex and computationally expensive numerical models.[6,7]

One of the powerful up-to-date numerical model, answering the above requirements, is the mesoscale weather research and forecasting model WRF, designed at the National Center for Atmospheric Research (USA).[8,9] The model is in open access; therefore, recent WRF-based investigations began in Russia[10] and showed it to be prospective in use.

This work describes our study, based on the WRF model modification WRF-CHEM [Ref. 11], which is a specially-purposed WRF variation, taking into account transfer of atmospheric pollutants (aerosols and gases) and their chemical transformations. For today, nobody use WRF-CHEM for atmospheric researches in Russia, though this model gives more possibilities to study real polluted air and is of interest.

Study description

We have considered nonstationary mesoscale meteoprocesses, including pollutant transfer in the East-European region of Russia (55.6°N, 51°E, Tatarstan), and conducted 3-dimensional numerical modeling of the atmospheric layer dynamics up to heights of about 20 km for areas with horizontal sizes 800×600 km, 100×100 km, and 15×15 km. The modeled volume was approximated by discrete grids of 80×60, 100×100, and 50×50 nodes, respectively, in the horizontal plane and had 31 vertical layers.

The boundary conditions were set with accounting for specific features of the territory: actual height relief, type of underlying surface, features of heat and moisture exchange between the underlying surface and the ground atmosphere. We used high-resolved (30″ step) maps of the actual underlying surface.

0235-6880/08/01 59-05 $02.00

The modeling includes the numerical integration of the hydrodynamic and transfer equations with WRF-CHEM-based parameterization of some additional important atmospheric processes.

The WRF-CHEM model, like WRF, allows air flow hydrodynamics to be calculated on the base of compressible Navier–Stokes equations to not-hydrostatic approximation, represented in curvilinear coordinates.[12] Integration is carried out by the method of explicit division into the gravitation and acoustic wave modes.[13] Model is applicable in present-day powerful computer systems, supports computational parallelism, realizes numerical representation of physics of different atmospheric processes.

An original part of WRF-CHEM realizes numerical integration of the atmospheric pollutant transfer (aerosols and gases) and their chemical transforming by the RAD2 [Ref. 14] and MADE [Ref. 15] models, including SO_2, NO, NO_2, NO_3, CO, and other pollutants (30 classes of anthropogenic emissions). Admixture sedimentation on the underlying surface is considered.[16] Parameterization of biogenic sources by means of the land-use map with the help of the Hanter model[17] is used. The model allows calculations for an arbitrary spatial system of pollutant sources (including ones located above the surface) with accounting for their time–power dependence (with 1-hour step).

Results of global final analysis of the 3D EMC modeling were used as initial and boundary conditions.[18] These results[19] for the last year are available on the UCAR/NCAR site. They have a data resolution of 1° and an interval of 6 h. To set the initial background concentration of different pollutants, idealized profiles are used.

To take into account peculiarities of individual atmospheric processes, we tested many numerical schemes in calculations for all seasons. The analysis of calculation and experimental results have shown that the most optimal for our conditions are schemes, using Lin et al. microphysics scheme, Kain–Fritsch parametrization of cumulus cloud effect and convection, Noah Land Surface Model, Yonsei University (YSU) model of atmospheric boundary layer, Rapid Radiative Transfer Model (RRTM), and Dudhia scheme of shortwave radiation. Surface layer effects were calculated on the base of Monin–Obukhov similarity theory.

The dynamics of nonuniform structure of 3D fields of wind velocity, temperature, humidity (including phase states), and pollutant concentration has been obtained from the calculations. Such results give a wide field for comprehensive spatio-temporal investigation of the ground atmosphere.

The distributed computations were made using the computer cluster of the Physical department at the Kazan State University.

Modeling results and comparison with experimental data

The model and experimental results for the summer of 2005 are shown in Fig. 1.

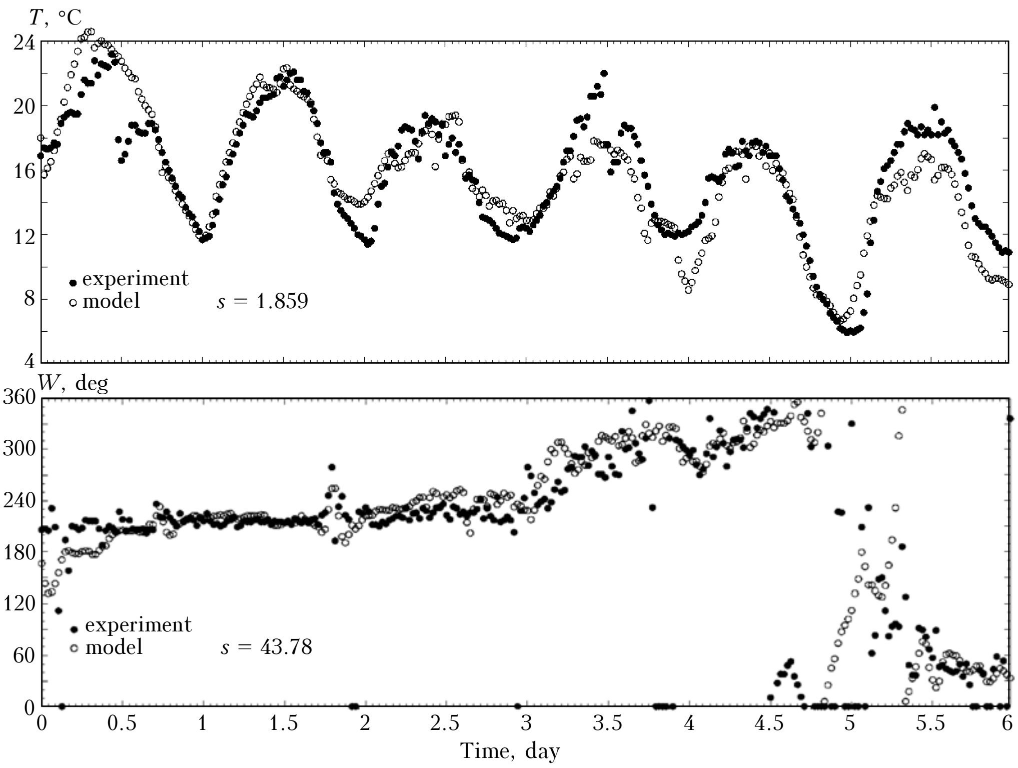


Fig. 1. Comparison of the model results with experimental data for air temperature and wind direction at the Aznakaevo station. Time reckoning is from 03:00 of July 1, 2005 with the 30-min interval; *s* is rms deviation of series.

RMS deviations of the model results from experimental (by experimental series with the 30-min step) for different seasons are given in Table.

Parameter	Summer	Winter	Spring	Autumn
Temperature, °C	1.775	3.592	2.678	1.472
Relative humidity, %	9.794	11.17	30.79	9.36
Wind direction, degree	37.41	18.8	49.32	23.87

The comparison results in Fig. 1 show a good agreement with experimental ones. This especially concerns large-scale time variations (4–6 hours and more). The daily variations are clearly pronounced on the humidity (not shown) and temperature plots with superimposed irregular distortions. A good agreement between the model and experiment is seen on the wind direction plots, especially in the period of steady and slow wind direction changing with time. At the end of the period, sharp change of wind direction is observed. Model predictions are less correct in such adverse weather conditions. Comparison results, generalized over the computation array and seasons, show satisfactory agreement between the model and experiment.

Different behavior of time series for scales less than 4–6 hours can be related to both insufficient equivalence of numerical schemes of individual physical processes and insufficient spatial resolution of the model, which results in impossibility of full resolution of delicate and small-scale physical processes. The question needs in additional study, particularly, in model computation at a high-power computer cluster and at a high spatial resolution.

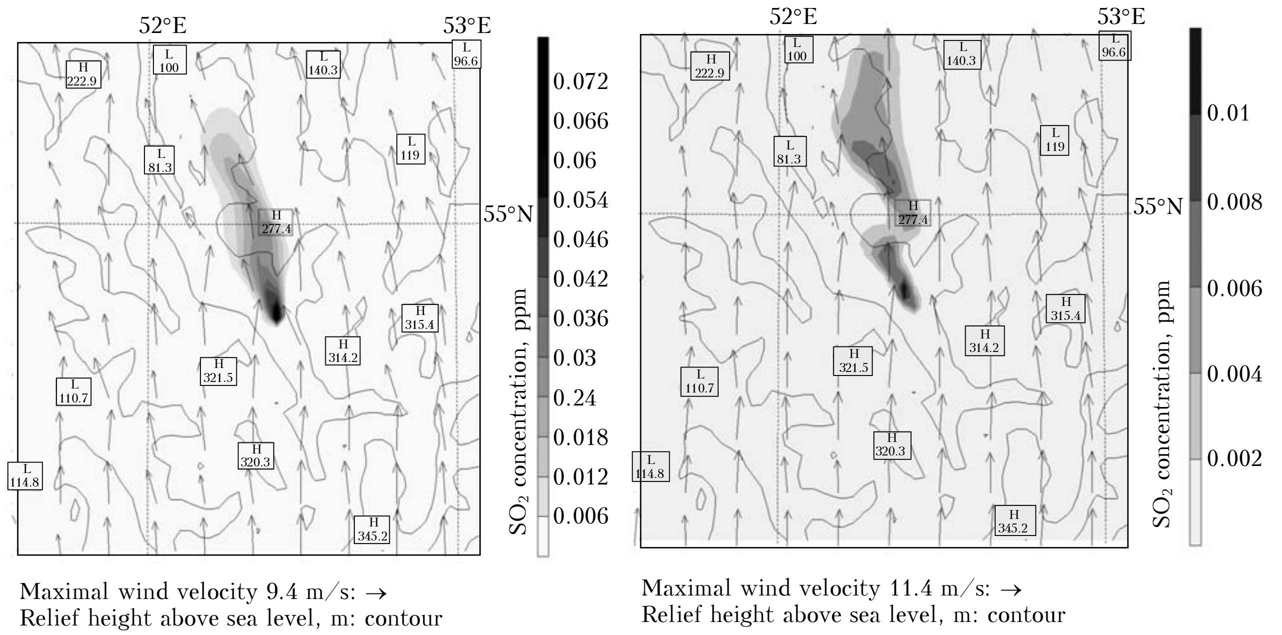
Forecast of local nonuniform structure of atmospheric pollutants

Spatial fields of trace gases and aerosol mass concentrations have been modeled. Figure 2 shows the modeling results of SO_2 pollutant propagation from a permanent-output source onto the territory of 100×100 km centered at Al'met'evsk town (54.9°N, 52.3°E). The relief, wind velocity field, and pollutant concentration level are shown.

A source of a permanent emission of 550 kg/h was modeled. The source corresponds to a real local industrial enterprise, which emission consists 99% of SO_2 among all industrial enterprises in the town. Pollutant propagation with airflow is evident in the shown horizontal shear. The pollutant concentration decreases with distance.

An important result of the study is formation of a nonuniform structure of the pollutant concentration field, a change with height of not only the mean pollutant concentration but its spatial structure as well. The most pronounced quasi-periodical nonuniform structure of pollutant concentration is formed within the region of high concentrations. The longitudinal horizontal scale is 15–25 km, transversal horizontal scale is 4–8 km, and vertical one is 100–200 m (much less than the horizontal one).

The obtained results correspond to the experimental spatial inhomogeneity scales of trace gases concentrations, obtained with the network of atmosphere monitoring stations in Al'met'evsk town.[4]



a *b*

Fig. 2. SO_2 concentration at a height of 30 (*a*) and 70 m (*b*) 120 min later the emission beginning.

To model aerosol propagation from several sources in a small industrial town, the area of 15×15 km around Al'met'evsk has been considered, allowing the modeling with the 300-m horizontal discrete step and the distinguishing emissions from several small enterprises. The height difference in this local area is about 250 m.

Total aerosol propagation with time can be traced in the given horizontal and vertical shears (Figs. 3 and 4).

Among 22 permanent-emission sources (the most pronounced emission is 61 kg/h), three are most noticeable. One of them is located at the area edge, hence, its emission were carried out of the area.

Aerosol propagation to a height of 70–120 m is evident from the horizontal shears of different heights for the same time moment (see Fig. 3); where the concentration decreases by *e* time in comparison with the surface region. The emission trace bending due to nonuniformity of the wind velocity field, caused by the relief, is seen.

Figure 4 shows the vertical shear along the emission trace and perpendicular shear, revealing the complex vertical structure of the background aerosol concentration distortions. Two emission sources are seen in the longitudinal shear, as well as the height structure of the absolute aerosol concentration. As it was expected, the speed of pollutant propagation in the surface layer increases with distance and, according to the numerical forecast for our case, reaches its maximum at a height of 70 m. As is seen from the comparison with shears at other time points (are not shown here), wind velocity inhomogeneities are spatially coherent, and their movement with time is noticeable.

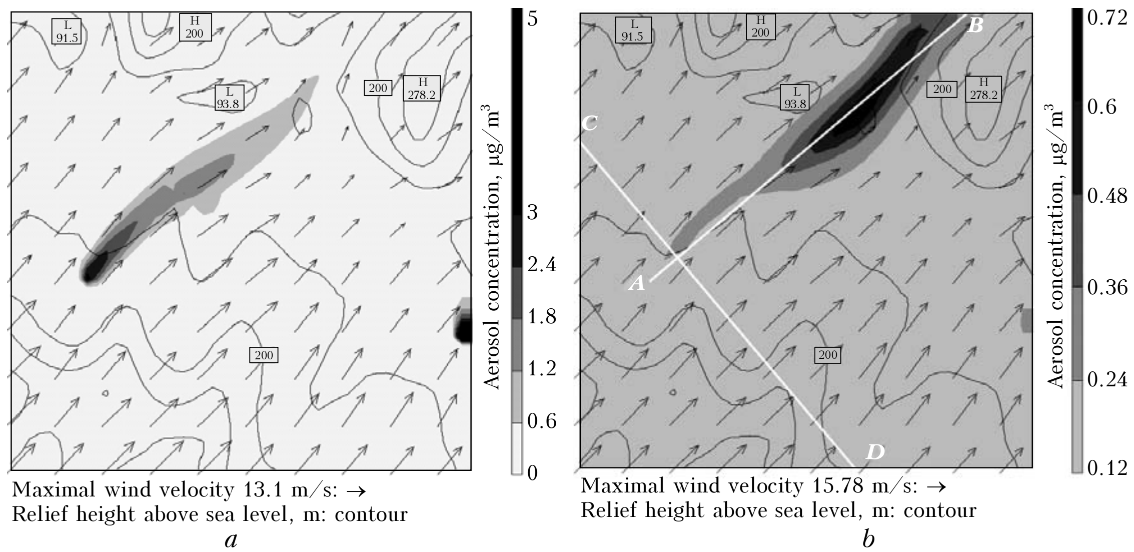


Fig. 3. Aerosol concentration at a height of 30 (*a*) and 70 m (*b*) 60 min later the emission beginning.

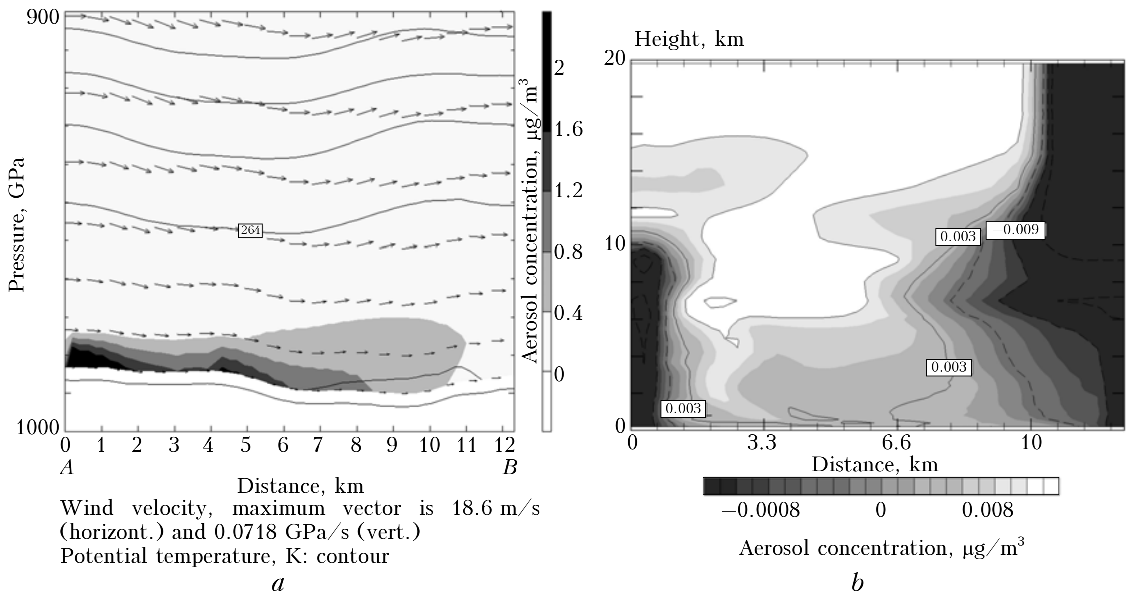


Fig. 4. Vertical slices *AB* and *CD* (see Fig. 3) 20 min later the emission beginning: absolute aerosol concentration (*a*) and the departure from the mean height profile (*b*).

Conclusion

Based on the WRF-CHEM model for computing complex dynamics of the real atmosphere and processes of pollutant transfer over the East-European region of Russia, a numerical model has been worked out with accounting for local geographic features: real relief and high-resolution land-use maps were used, optimal numerical schemes of atmospheric processes were chosen.

The model allows one to obtain a detail 3D-dynamics of fields of meteoparametrs and pollutant concentrations. On the base of the model, numerical modeling for the geographic region under study has been carried out for the first time. The results show complex vertical and horizontal structures of formed inhomogeneities in the pollutant concentration field.

A quasi-periodic nonuniform structure of wind velocity and pollutant concentration fields is formed. The longitudinal horizontal scale is 15–25 km, transversal scale is 4–8 km, and vertical one is 100–200 m (much less than the horizontal one). Drift of the inhonogeneities with time has been revealed. These results correspond to the experimental data on mesoscale atmospheric inhomogeneities of trace gases concentrations, obtained earlier with the network of atmosphere monitoring stations in the Al'met'evsk town. The model, as experimental results, confirms an orographic nature of local atmospheric inhomogeneities of meteoparameters and surface pollutants even for a quasi-plane relief.

The model has shown a good agreement with experimental data, therefore, it is suitable for a broad spectrum of scientific and applied problems, as well as in the forecast of pollutant transfer and propagation. As compared with experimental results, not only fine horizontal structure, but also vertical structure of lower atmosphere can be obtained, including the pollutant concentration.

Acknowledgements

This work is partially supported by the Russian Foundation for Basic Research (Grant No. 04–05–64194) and RAS (Government Contracts Nos. 06–6.3–13 and 09–9.5–32).

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