Modeling of admixture transport and transformation in the atmosphere based on the Models-3 system

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Main peculiarities of the information–prediction system of the third generation Models-3 designed at the U.S. Environmental Protection Agency for the problems of predicting the atmospheric air quality are considered. The calculation results obtained with this system are presented.

Introduction

Many mathematical models used both in theoretical and applied investigations have been developed for describing evolution of admixtures in the atmosphere. Nevertheless, the questions are still urgent which are related to the creation of mathematical models, which are of practical value in solving the problems in predicting the quality of atmospheric air and its optical properties. The information–prediction system of third generation (the Models-3 system) was developed in nineties at the U.S. Environmental Protection Agency as a tool for supporting the decision-making on the environmental protection by the governmental agencies.[9–13,17,18] It seems that the system is now among the most competitive in the world.

The principal peculiarities of the Models-3 system are described in this paper, and its capabilities for solving the problems of predicting the quality of atmospheric air and its optical properties are demonstrated.

Principal components of the system

The functional block-diagram of the Models-3 system is shown in Fig. 1. One of its principal components is the meteorological modeling system that generates the meteorological fields (horizontal and vertical components of wind velocity, pressure, humidity of air, characteristics of cloudiness and precipitation, fluxes of heat, moisture and momentum, fluxes of short wave and long wave radiation).

The third version of the system of fifth generation MM5 created at the National Center for Atmospheric Research (NCAR) in cooperation with the University of Pennsylvania[19,20,24] is used for modeling (prediction) of meteorological fields. The MM5 system provides for non-hydrostatic dynamics and for a possibility of using the scheme of 4D adoption of data at numerical prediction[29]; it has a great number of schemes of parameterization of the subgrid physical processes selected by a researcher based on the problem stated and spatial scale of the processes under consideration. It allows one to construct the telescopic model (up to 9 enclosed grids) with one-way or two-way interaction between the grids. The ratio of the horizontal steps of the grids should be 1:3.

Let us consider the principal blocks of the MM5 system (Fig. 1). The TERRAIN block provides for referencing the grids of the model to geographic coordinates by means of setting the horizontal size (number of nodes) and spatial resolution of the grid of a regional model, latitude and longitude of the central point of the regional grid, the used cartography projection (polar, stereographic, Lambert or Mercator, that makes the model to be applicable at any latitude), number of enclosed grids, their size, horizontal resolution and the position of the left lower node relative to the left lower node of the higher-level grid. This subroutine serves also for the formation of the data on the relief of the underlying surface based on the databases existing in the MM5 system. To set the relief and the properties of the underlying surface, one can use global topographic data of different resolution from 1 to 30°.

The REGRID subroutine is aimed at setting the first approximation of the meteorological fields by means of archive data or the data of the preceding prediction. The data of NCAR reanalysis or European Center of weather prediction, or global data of NCAR after the procedure of adoption, or the data of regional analysis and prediction are taken as archive data. All calculations are repeated for each grid. Files containing the data on temperature of the ocean surface and the data on snow cover are also formed in the frameworks of the REGRID.

Objective analysis (OA) of meteorological fields is performed in the subroutine RAWNIS. The data obtained in the subroutine REGRID are used as the first approximation. Synoptic data are also used in making OA, as well as the data on geopotential, wind, and relative humidity of air at the following isobaric surfaces: 1000, 850, 700, 500, 400, 300, 250, 200, 150, and 100 hPa.

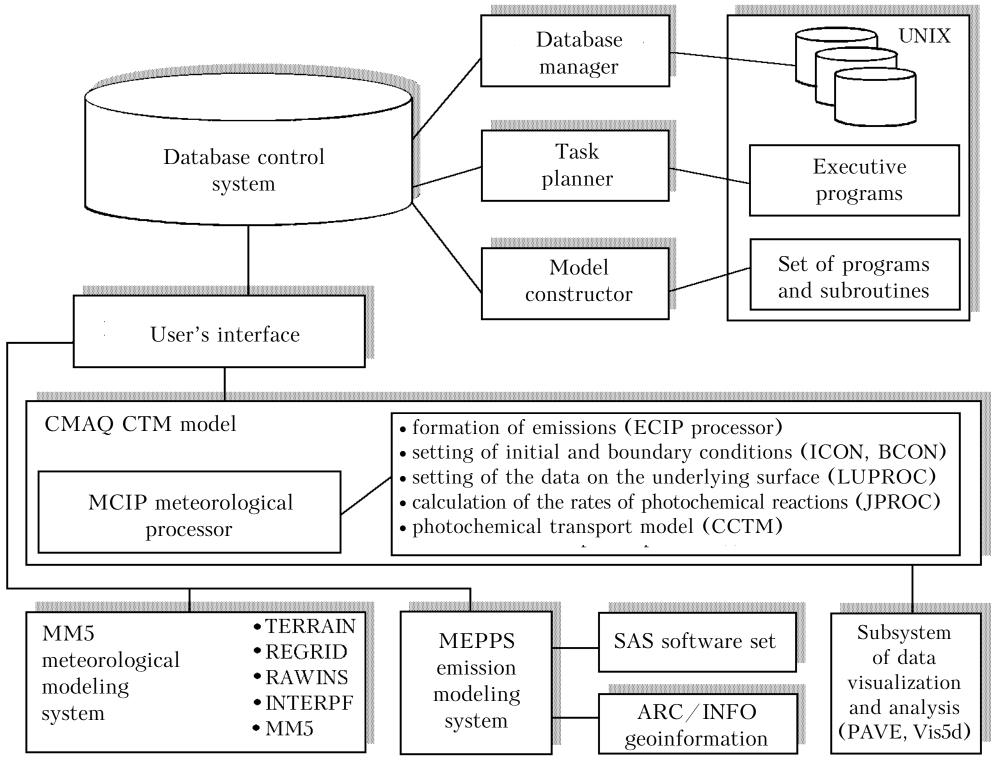

Fig. 1. Structure of the Models-3 system.

Four variants of realization of the OA scheme are provided. They are the Cressman scheme,[15] elliptic scheme,[3] its improved variant ("banana" scheme[3]), and the scheme based on the multidimensional quadratic interpolation.[27] After OA the data are interpolated to the additional p-levels, which the researcher has set.

The initial and boundary conditions (side, lower, and upper) for all grids of the model are formed in the INTERPF module. The data are interpolated from the isobaric levels to the σ-surfaces and the shattered horizontal B-grid. A researcher determines the number of levels. In addition, this module initializes the model.

The MM5 module itself is, in fact, aimed at forecasting (modeling) of the meteorological processes. The non-hydrostatic model used for this purpose allows one to vary the horizontal resolution from hundreds of meters to tens kilometers. The system of equations of the model is written in the σ-coordinate system ($\sigma = (p - p_t)/(p_s - p_t)$) and includes three equations of motion, equation of heat influx, equation for prediction of pressure, and the equation of the moisture transfer (here we write it):

$$\frac{\partial u}{\partial t} + \frac{m}{p}\left(\frac{\partial p'}{\partial x} - \frac{\sigma}{p^*}\frac{\partial p^*}{\partial x}\frac{\partial p'}{\partial \sigma}\right) =$$

$$= -\mathbf{V}\,\nabla u + v\left(f + u\frac{\partial m}{\partial y} - v\frac{\partial m}{\partial x}\right) - e\,w\cos\alpha - \frac{uw}{r_0} + D_u,$$

$$\frac{\partial v}{\partial t} + \frac{m}{p}\left(\frac{\partial p'}{\partial y} - \frac{\sigma}{p^*}\frac{\partial p^*}{\partial y}\frac{\partial p'}{\partial \sigma}\right) =$$

$$= -\mathbf{V}\,\nabla v - u\left(f + u\frac{\partial m}{\partial y} - v\frac{\partial m}{\partial x}\right) + e\,w\sin\alpha - \frac{vw}{r_0} + D_v,$$

$$\frac{\partial w}{\partial t} + \frac{\rho_0}{\rho}\frac{g}{p^*}\frac{\partial p'}{\partial \sigma} + \frac{g}{\gamma}\frac{p'}{p} = -\mathbf{V}\,\nabla w + g\frac{p_0}{p}\frac{T'}{T_0} - \frac{gR_d}{c_p}\frac{p'}{p} +$$

$$+ e\,(u\cos\alpha - v\sin\alpha) + \frac{u^2 + v^2}{r_0} + D_w,$$

$$\frac{\partial T}{\partial t} = -\mathbf{V}\,\nabla T + c_p)\left(\frac{\partial p'}{\partial x} + \mathbf{V}\,\nabla p' - \rho_0\,g w\right) + \frac{\dot{Q}}{c_p} + \frac{T_0}{\theta_0}D_0,$$

$$\frac{\partial p'}{\partial t} - \rho_0\,g w + \gamma p \nabla\mathbf{V} = -\mathbf{V}\,\nabla p' + \frac{\gamma p}{T}\left(\frac{\dot{Q}}{c_p} + \frac{T_0}{\theta_0}D_0\right).$$

The advective and divergent terms have the following form:

$$\mathbf{V}\,\nabla A \equiv mu\frac{\partial A}{\partial x} + mv\frac{\partial A}{\partial y} + \dot{\sigma}\frac{\partial A}{\partial \sigma}\,;$$

$$\nabla\mathbf{V} = m^2\frac{\partial}{\partial x}\left(\frac{u}{m}\right) - \frac{m\sigma}{p^*}\frac{\partial p^*}{\partial x}\frac{\partial u}{\partial \sigma} + m^2\frac{\partial}{\partial y}\left(\frac{v}{m}\right) -$$

$$- \frac{m\sigma}{p^*}\frac{\partial p^*}{\partial y}\frac{\partial v}{\partial \sigma} - \frac{g\,\rho_0}{p^*}\frac{\partial w}{\partial \sigma}\,,$$

where

$$\dot{\sigma} = -\frac{\rho_0\,g}{p^*}\,w - \frac{m\sigma}{p^*}\frac{\partial p^*}{\partial x}\,u - \frac{m\sigma}{p^*}\frac{\partial p^*}{\partial y}\,v\,;$$

$e = 2\Omega\cos\lambda$; λ is latitude; $\alpha = \varphi - \varphi_c$

(φ is the longitude, φ_c is the longitude of the central point of the grid): r_0 is the mean Earth's radius, $\dot{Q}$ is the heat influx, $p^* = p_s - p_1$. Other notations are the generally accepted ones.

Numerical solution of the equations of the model is achieved by means of the method of splitting the physical processes. The subsystem describing slowly moving waves is integrated using the scheme of central differences.[7] To solve the subsystem describing the fast waves motion, the semi-implicit numerical algorithm is applied. The equations of the model are approximated in the horizontal plane within the second-order accuracy on the Arakava B-grid.

The relaxation procedure[16] is used for setting the side boundary conditions at the boundaries of the regional model:

$$\left(\frac{\partial \alpha_M}{\partial t}\right)_n = F(n)\, F_1(\alpha_{LS} - \alpha_M) - F(n)\, F_2\, \nabla^2(\alpha_{LS} - \alpha_M),$$

where $F_1 = 0.1/\Delta t$; $F_2 = (\Delta x)^2/50\Delta t$; $F(n)$ is the weighting function depending on the number of the grid nodes n counted from the side boundary, α_{LS} and α_M are the values of the considered function calculated based on the data of global modeling and the data of the model, respectively.

There is a possibility of using different variants of substituting the side boundary conditions for the enclosed grids: constant, relaxation procedure, method of weighted tendencies, method of damping by absorption, free influx/outflux.[16,24,28]

The model contains quite a great number of the schemes of parameterization for description of the physical processes on the subgrid scale. Eight schemes of parameterization[1,2,4,5,19,24,26,31] provide for description of convective processes, each of them having its own domain of applicability. In the case when the horizontal scale is 5 km or less, the convective processes are not parameterized, but modeled explicitly. Six schemes[6,8,24,32] are used for description of the processes occurring in the planetary boundary layer (PBL) of the atmosphere. Selection of the specific scheme depends on the number of levels assumed by the model for the PBL. Then it is possible to calculate temperature and humidity of soil based on the solution of 1D equations of heat and humidity transfer in soil.[20]

Five schemes of parameterization are provided in the model for making calculations of the radiation fluxes and heat influxes: the simplest scheme, in which cooling of the atmosphere depends only on temperature, to multi-spectral schemes taking into account interaction of radiation fluxes with clouds.[24] Microphysical processes and phase heat influxes are described by means of eight schemes which also are characterized by different degree of detailing.[24]

The emission modeling system MEPPS is also one of the principal components of the Models-3 system. It is intended for calculation of emissions – power and intensity of sources of emission of different ingredients into the atmosphere taking into account meteorological conditions and the considered geographic region. The system operates with the database of the sources of pollution, which are divided into point, aerial (including the sources of biogenic origin), and mobile. When creating this database for the territory of North America, the Environmental Protection Agency has done a lot of inventory work on all types of sources. Numerous data of Federal Services and Agencies, services and agencies of different states, cities, and enterprises were also used. Inventory of mobile sources was based on the statistical data on moving of motor vehicles of different categories on the roads of the USA, Canada, and Mexico. MEPPS is supported by the ARC/INFO geoinformation system and by SAS (Statistical Analysis System) applied software, by means of which the data on emissions are processed and the parts of the MEPPS subsystem are controlled.

The central block of the Models-3 is the CMAQ CTM subsystem (Community Multiscale Air Quality Chemical Transport Modeling System). All necessary data used by the chemical transport model (CTM) for modeling the processes of evolution of pollution and their sedimentation taking into account chemical transformations are prepared by this subsystem, as well as numerical modeling is performed.

The CMAQ subsystem has the modular structure (see Fig. 1). The LUPROC (Land-Use Processor) module serves for the formation of data of high resolution on the underlying surface and their referencing to the set grid. Then these data are used in the MCIP (Meteorology-Chemistry Interface Processor) module for calculation of the parameters of the planetary boundary layer of the atmosphere and the rates of washing out of different substances from the atmosphere. Formation of the files containing the data on meteorological parameters relative to the grid used in the chemical transport model (CTM) occurs in the MCIP module, as well as calculation of the parameters of cloudiness, rates of dry and wet washing out, turbulent exchange coefficients, and the parameters of interaction of the admixtures with the underlying surface.

The ECIP (Emission-Chemical Interface Processor) module generates hourly 3D fields of pollution using the output files of the MEPPS block. The ICON and BCON modules form the initial and boundary conditions for chemical transport model. The rates of chemical reactions are calculated in the JPROC block taking into account the vertical profiles of the shortwave solar radiation.

Principal equation of the chemical transport model is written in the generalized coordinate system $(\hat{x}_1, \hat{x}_2, \hat{x}_3, \hat{t})$ and has the form[9]

$$\frac{\partial(\varphi_i\, J_\xi)}{\partial t} + m^2\, \nabla_\xi \left(\frac{\varphi_i\, \hat{\mathbf{V}}_\xi J_\xi}{m^2}\right) + \frac{\partial(\varphi_i\, \hat{u}_3 J_\xi)}{\partial \hat{x}_3} +$$

$$+ m^2 \frac{\partial}{\partial \hat{x}^1}\left(\frac{\rho J_\xi}{m^2}\, \hat{F}^1_{q_i}\right) + m^2 \frac{\partial}{\partial \hat{x}^2}\left(\frac{\rho J_\xi}{m^2}\, \hat{F}^2_{q_i}\right) + \frac{\partial}{\partial \hat{x}^3}(\rho J_\xi \hat{F}^3_{q_i}) =$$

$$= J_\xi R_{\varphi_i}(\varphi_1, \ldots, \varphi_N) + J_\xi Q_{\varphi_i} + \left.\frac{\partial(\varphi_i J_\xi)}{\partial t}\right|_{\text{cloud}} + \left.\frac{\partial(\varphi_i J_\xi)}{\partial t}\right|_{\text{aero}} + \left.\frac{\partial(\varphi_i J_\xi)}{\partial t}\right|_{\text{ping}},$$

here φ_i is the specific concentration of the ith admixture, J_ξ is the Jacobian transform depending on the type of vertical coordinate (Table 1), R_{φ_i} is the term describing the change in the concentration of the ith admixture due to chemical transformations, $q_i = \varphi_i/\bar{\rho}$; Q_{φ_i} is the function describing the sources/sinks of the ith admixture, and $\hat{F}^k_{q_i}$ is the turbulent flux of the ith admixture:

$$\hat{F}^1_{q_i} = m\, F^1_{q_i}, \quad \hat{F}^2_{q_i} = m\, F^y_{q_i},$$

$$\hat{F}^3_{q_i} = \left(\frac{\partial \hat{x}_3}{\partial x}\right) F^x_{q_i} + \left(\frac{\partial \hat{x}_3}{\partial y}\right) F^y_{q_i} + \left(\frac{\partial \hat{x}_3}{\partial z}\right) F^z_{q_i}\,.$$

Table 1

Vertical coordinate	Definition	Vertical velocity	Jacobian
z*		$w = \frac{\mathrm{d}z}{\mathrm{d}t}$	1
$\sigma_{\overline{Z}}$	$\sigma_{\overline{Z}} = H\frac{z - z_{\text{sfc}}}{H - z_{\text{sfc}}}$	$\frac{\mathrm{d}\sigma_{\overline{Z}}}{\mathrm{d}t}$	$\frac{H - z_{\text{sfc}}}{H}$
σ_Z	$\sigma_Z = \frac{z - z_{\text{sfc}}}{H - z_{\text{sfc}}}$	$\frac{\mathrm{d}\sigma_{\overline{Z}}}{\mathrm{d}t}$	$H - z_{\text{sfc}}$
$1 - \sigma_{p_0}$	$\sigma_{p_0} = \frac{p_0 - p_T}{p_{\text{os}} - p_T}$	$-\frac{\mathrm{d}\sigma_{p_0}}{\mathrm{d}t}$	$\frac{p_{\text{os}} - p_T}{\rho_0 g}$
$1 - \sigma_{\tilde{p}}$	$\sigma_{\tilde{p}} = \frac{\tilde{p} - p_T}{\tilde{p}_s - p_T}$	$-\frac{\mathrm{d}\sigma_{\tilde{p}}}{\mathrm{d}t}$	$\frac{\tilde{p}_s - p_T}{\tilde{p} g}$

* Geometric height.

The last three terms of the CTM model describe, respectively, interaction of the admixture with clouds, generation of the aerosol component, and the rate of the change of substances due to the diffusion of admixtures at the first stage of evolution, when the admixture is not "caught" by the grid of the model.

The system provides for twelve variants of describing the processes of chemical interaction of the gaseous components on the basis of the mechanisms CB–IV (Carbon Bond)[23] and RADM (Regional Acid Deposit Model) of the second version.[30] The CB–IV mechanism used by the CMAQ system includes 36 gaseous components and 93 chemical reactions, including 11 photochemical reactions. The RADM2 mechanism describes 57 gaseous components and 158 chemical reactions, 21 of which are photochemical reactions. Interaction with atmospheric moisture and generation of aerosol are taken into account when describing chemical reactions.

Chemical processes in the atmosphere are described by the system of nonlinear ordinary differential equations, which are referred to the class of "hard" equations according to their properties. Two algorithms are used for numerically solving this system – the implicit one with the automatic selection of the time step and control of the error of calculations,[22,25] and the explicit one, which is less accurate, but, nevertheless, provides for a sufficient accuracy while requiring less computational burden.[17,18]

The Models-3 system has very suitable and flexible interface, by means of which the processes of data preparation, processing and visualization, assemblage of the model of the required configuration, preparation of the task, etc., are controlled. The function of controlling the data, meta-data, and programs inside the system is rested on the object-oriented database control system, which also provides for the interaction of the executed blocks of the Models-3 system taking into account the project prepared by a researcher. The project (or task) is stated by means of the Task Planner and the Model Constructor.

Now the CTM model allows one to use the grid with the horizontal resolution of 108, 36, 12, and 4 km, and the number of vertical levels is from 6 to 30. The researcher can increase (decrease) the quantity of the considered chemical and aerosol components, add and modify chemical and photochemical reactions at his/her discretion.

Results of numerical modeling

The Models-3 system is realized on the following calculation platforms – Cray, Sun, SGI, HP, IBM, and DEC. The results discussed below are obtained at the Sun Ultra 10 computer.

The MM5 model used for numerical modeling had the following configuration. The size of the grid of the regional model is 75×64 nodes (on the x and y axes, respectively) with the resolution of 108 km. The central point of the grid had the following geographic coordinates: 90°W and 40°N. The Lambert cartographic projection was used. The enclosed grid had the size of 60×56 nodes with the step of 36 km. The quantity of vertical levels was equal to 30. The output file of the MM5 model at such a configuration had the size of 12.2 Gbyte/day.

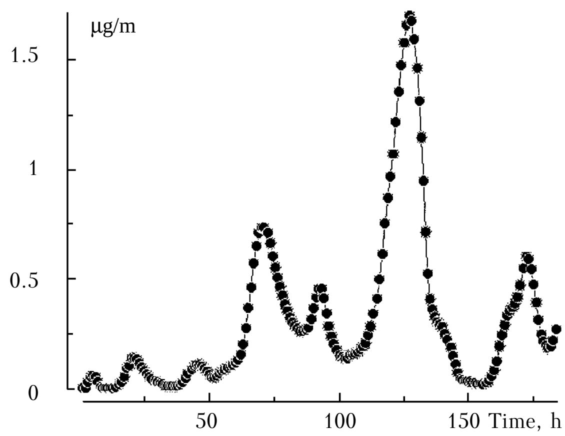

Fig. 2. Temporal behavior of the volume number density of cumulative fraction of sulfate aerosol in the near-ground layer of the atmosphere (the data are averaged over the grid of the CCTM model).

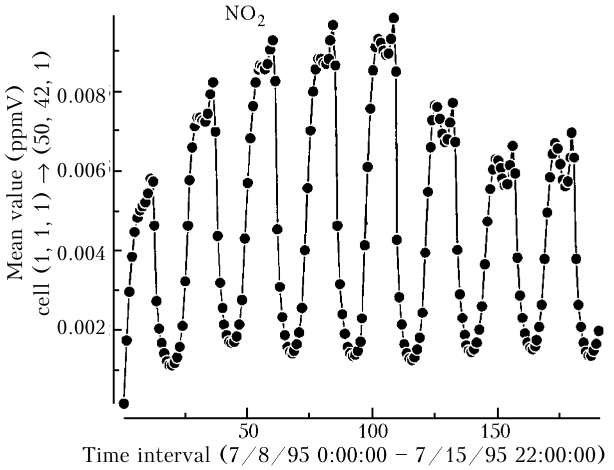

Fig. 3. Temporal behavior of the content of nitrogen dioxide NO_2 in the near-ground layer of the atmosphere (the data are averaged over the grid of the CCTM model).

Convective processes were described by the Kuo scheme (regional model) and the Kain–Fritch scheme[26] (enclosed model). The Blackadar[6] scheme with high resolution was used for PBL parameterization. Clouds and precipitation were modeled by means of the scheme which describes the phase transformations on microphysical level and formed the mixed phase.[19] A sufficiently detailed and complicated scheme was applied for making calculations of the radiative heat influxes taking into account interaction of the radiation fluxes with clouds.[24]

The grid of the CTM model had the size of 50×42 with the resolution of 36 km. The quantity of vertical levels was 30, and the upper boundary of the model was at the level of the tropopause.

Integration was performed over 8 days for the period of July 8 to 15, 1995. These dates were taken in connection with the fact that the NARSTO observation experiment was carried out in North America in this time. The data of this experiment can be used for verification of the model.

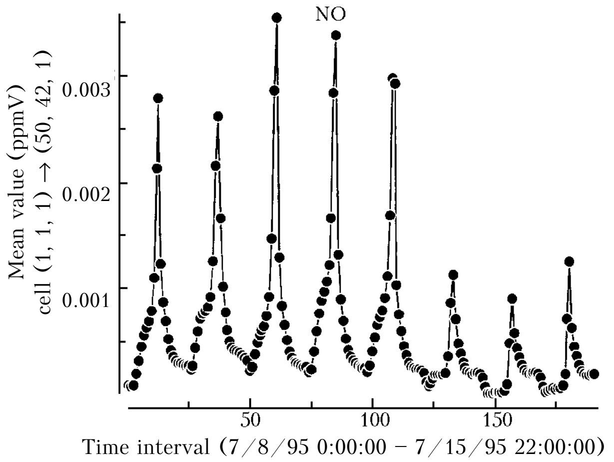

Fig. 4. Temporal behavior of nitrogen oxide NO in the near-ground layer of the atmosphere (the data are averaged over the grid of the CCTM model).

Let us present some results of numerical simulation. Temporal behavior of the volume number density of the cumulative fraction of sulfate aerosol in the near-ground layer of the atmosphere is shown in Fig. 2. Temporal behaviors of nitrogen oxide and dioxide in the near-ground layer of the atmosphere are shown in Figs. 4 and 3, respectively. Diurnal behavior of the atmospheric pollution by the aforementioned ingredients is well seen in these figures.

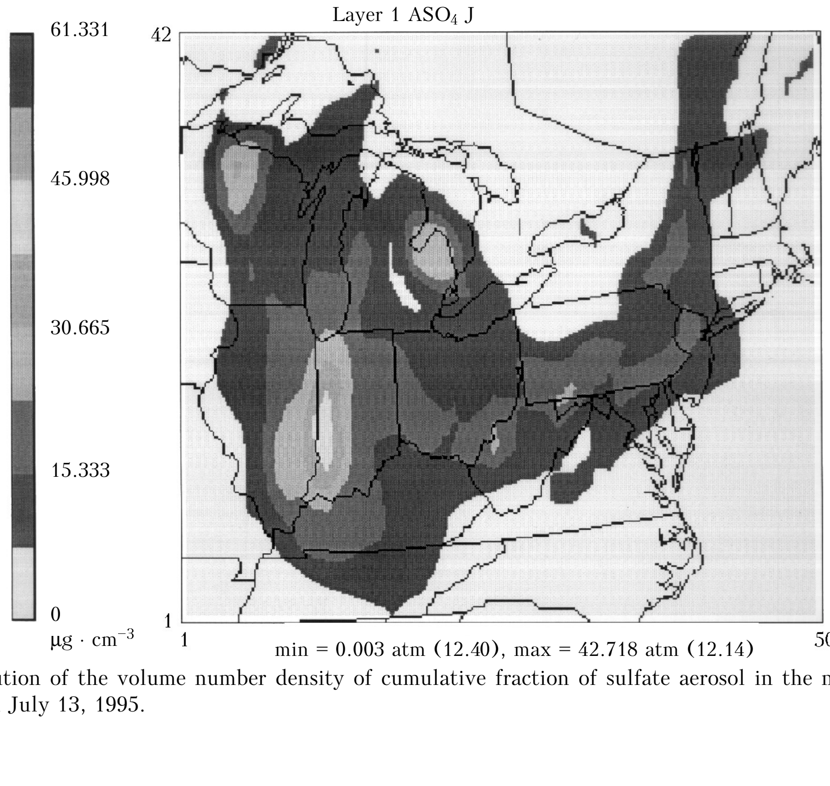

Fig. 5. Spatial distribution of the volume number density of cumulative fraction of sulfate aerosol in the near-ground layer of the atmosphere at 9 AM on July 13, 1995.

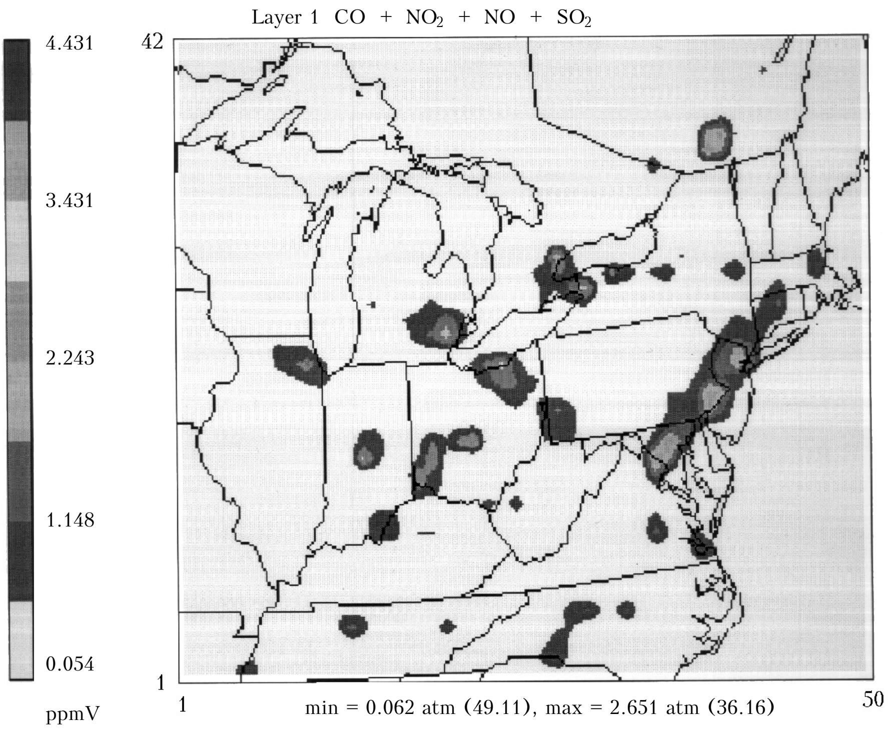

Fig. 6. Spatial distribution of the total contents of nitrogen oxides (NO and NO_2), carbon monoxide CO and sulfur dioxide SO_2 in the near-ground layer of the atmosphere at 11 AM on July 12, 1995.

Spatial distribution of the volume number density of cumulative fraction of sulfate aerosol at 9 AM on July 13, 1995 is shown in Fig. 5. Figure 6 shows the total contents of nitrogen oxides (NO and NO_2), carbon oxide CO and sulfur gas SO_2 at 11 AM on July 12, 1995. Clear correspondence between the sources of pollution and the modeled fields of the admixtures is seen in this figure. Optical properties of the atmosphere also can be assessed, because the data on the spatial distribution of natural and anthropogenic aerosol are contained in the output file of the model.

Conclusion

Now the system is tested, the database of the sources of atmospheric pollution is specified, and the models are adapted as applied to the territory of Canada. The Models-3 system can be used for solving different problems connected with the nature protection activity, including the prediction of the quality of atmospheric air, modeling of the consequences of technogenic catastrophes and crashes, elaboration of the policy in the field of nature protection activity, etc.

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Meteorological data were presented by NCAR that is responsible for supporting the databases.

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