

## SIMULATIONS OF VERTICAL DISTRIBUTION OF SULFURIC AND NITRIC COMPOUNDS CONCENTRATION IN THE BOUNDARY ATMOSPHERIC LAYER OVER SOUTHERN BAIKAL REGION

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*We present here the study of vertical distributions of the sulfuric and nitric compounds in the boundary layer of the atmosphere over Southern Baikal region. The study used a 3-D mathematical model for the dispersal and transformations of the pollutants assuming these processes to be unsteady and nonlinear. In the model study performed, we have considered only some typical, for this region, synoptic situations. The study enabled us to reveal the influence of the local orography on the dispersal of the contamination over the Lake Baikal region.*

Study of the atmospheric boundary layer pollution over Lake Baikal has become especially urgent in connection with the UNESCO decision to give the status of a world heritage region to Baikal. Mathematical modeling is an efficient approach to making such studies. An overview of the literature on the use of models to study the spread and transformations of aerosols and gaseous pollutants in the atmosphere near Baikal can be found in Refs. 1 and 2. A complex ecological model has been used to estimate the atmospheric pollution over Baikal region by the compounds of sulfur, nitrogen, and carbon in Ref. 3. However, the calculations were done on a grid with the horizontal step of 25 km, that made it impossible to take into account orography of the considered region in more detail. Recently, we have started the study of the dispersal and transformations of the sulfuric, nitric, and carbon compounds, coming from industrial objects of the Irkutsk-Cheremkhovo industrial region, as well as from Slyudyanka and Baikal'sk, using a 3-D Euler model<sup>4</sup> that assumes these processes to be unsteady and nonlinear. The model has been verified by the data of field measurements near Baikal in 1991–1992.<sup>1–2</sup>

In this paper, particular attention is paid to a more complete and efficient study of vertical distributions of these compounds and dust in the atmosphere over Southern Baikal by use of a mathematical model<sup>4</sup> based on numerical solution of the 3-D nonstationary semiempirical equation of turbulent diffusion and taking into account chemical reactions involving 82 substances. The choice of such a type of the model is caused by the following advantages.

1. Deterministic models have faster error decrease as compared with the statistical ones that are based on the Monte-Carlo method.

2. In contrast to Lagrange models, Euler models do not require integration over the spatial trajectory.

3. Euler models enable a more simple account of the orography. This is important for simulations concerning the region of Lake Baikal where the littoral area is occupied by high mountain ridges.

The details of the solution method may be found in Ref. 5.

We have numerically studied the dispersal of atmospheric pollution coming from industrial enterprises located in the South of Irkutsk region. In what follows we consider the emissions from industrial objects of Irkutsk, Angarsk, Usol'e-Sibirskoe, Cheremkhovo, Zima, Shelekhov, Slyudyanka, and Baikal'sk. We took into account the emissions of sulfur dioxide, nitrogen oxides, carbon oxide, and dust. Total power of the sources has been taken from Ref. 6. Other parameters of the sources have been presented by Irkutsk regional committee on ecology and use of natural resources.

For simulation we chose the integration domain of 400 by 250 km<sup>2</sup> area and 3-km height over the Lake Baikal surface. The steps in time were 300 s, while the horizontal step was 5 km, and the vertical one being set in the following way:

$$\Delta z = \begin{cases} 50 \text{ m} & \text{for } z \leq 500 \text{ m} \\ 100 \text{ m} & \text{for } 500 < z \leq 1000 \text{ m} \\ 500 \text{ m} & \text{for } z > 1000 \text{ m} \end{cases}$$

The coefficient of vertical turbulent diffusion was set to be equal to  $8 \text{ m}^2/\text{s}$ ; coefficients of horizontal turbulent diffusion were calculated by use of relations of semiempirical theory of turbulence:  $K_x = (V_0 + \sqrt{V^2/2}) \Delta x$ ;  $K_y = (V_0 + \sqrt{V^2/2}) \Delta y$ . Here  $K_x$ ,  $K_y$  are turbulent diffusion coefficients along the  $x$  and  $y$  axes, respectively;  $V$  is magnitude of the wind velocity vector;  $\Delta x$ ,  $\Delta y$  are grid steps along the horizontal coordinates  $x$  and  $y$ ;  $V_0 = 0.5 \text{ m/s}$ .

Four gaseous components are supposed to be emitted:  $\{\text{SO}_2, \text{NO}_2, \text{NO}, \text{and CO}\}$ . Background distributions<sup>3,8-11</sup> of the main components of the atmosphere (oxygen, nitrogen, and water vapor) and some trace gases are being taken as the initial conditions. The following substances are considered to be the yield of transformations:  $\{\text{OH}, \text{HCO}_3, \text{HO}_2, \text{SO}_3, \text{SO}_2^*, \text{SO}, \text{H}, \text{H}_2\text{O}_2, \text{N}_2\text{O}_5, \text{H}_2, \text{CO}_2, \text{H}_2\text{SO}_4, \text{O}, \text{HNO}_2, \text{HNO}_3\}$ .

Stoichiometric formulas of the reactions are presented in Ref. 4. Thus, the processes of the transfer, diffusion, and transformation are considered for 22 gaseous components and dust.

Numerical experiments were performed for different synoptic situations: calm, prevailing of local circulation, i.e., breezes, mountain-valley winds, joint action of local winds and background stream, pollutant transfer by north-west wind of different velocities.

Figure 1 presents vertical cross sections of the boundary layer for the atmosphere over Southern Baikal region at the north-west wind blowing at a speed of  $10 \text{ m/s}$ . Isolines of sulfur dioxide concentration are drawn by thin solid lines. The cross sections are made along the direction from north-west to the south-east. One of these passes through Angarsk and Irkutsk, the other is parallel to the first and passes through Shelekhov. The areas with local concentration maxima and minima are to be observed at windward and leeward slopes of the Primorskii mountain ridge, respectively. The values of  $\text{SO}_2$  concentration at the windward slopes exceed those of leeward slopes by an order of magnitude (Fig. 1a). The highest concentrations at the height of  $800 \text{ m}$  over the Baikal water table are observed over the top of the ridge and reach  $5 \mu\text{g}/\text{m}^3$ . In the other section (Fig. 1b), maximum concentrations at windward slopes exceed the corresponding concentrations at leeward slopes only by 4 fold. At the height of  $800 \text{ m}$ , extreme values of concentration are over the lake, they are a little bit higher than  $2 \mu\text{g}/\text{m}^3$ . It should be noted that the calculation do not take into account the initial ascending of the pollutants because its exact determination is connected with the basic difficulties in the choice of corresponding criteria.<sup>7</sup>

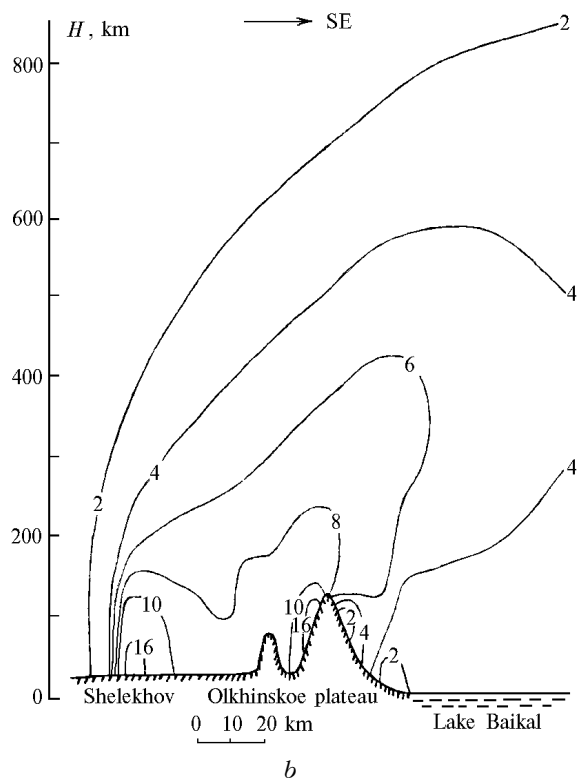
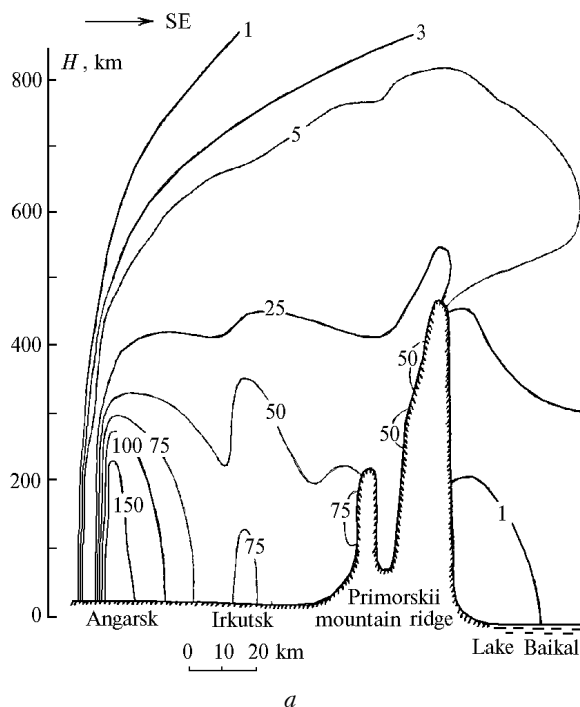


FIG. 1. Isolines of calculated sulfur dioxide concentrations,  $\mu\text{g}/\text{m}^3$ , in the cross sections Angarsk-Irkutsk (a), Shelekhov (b).

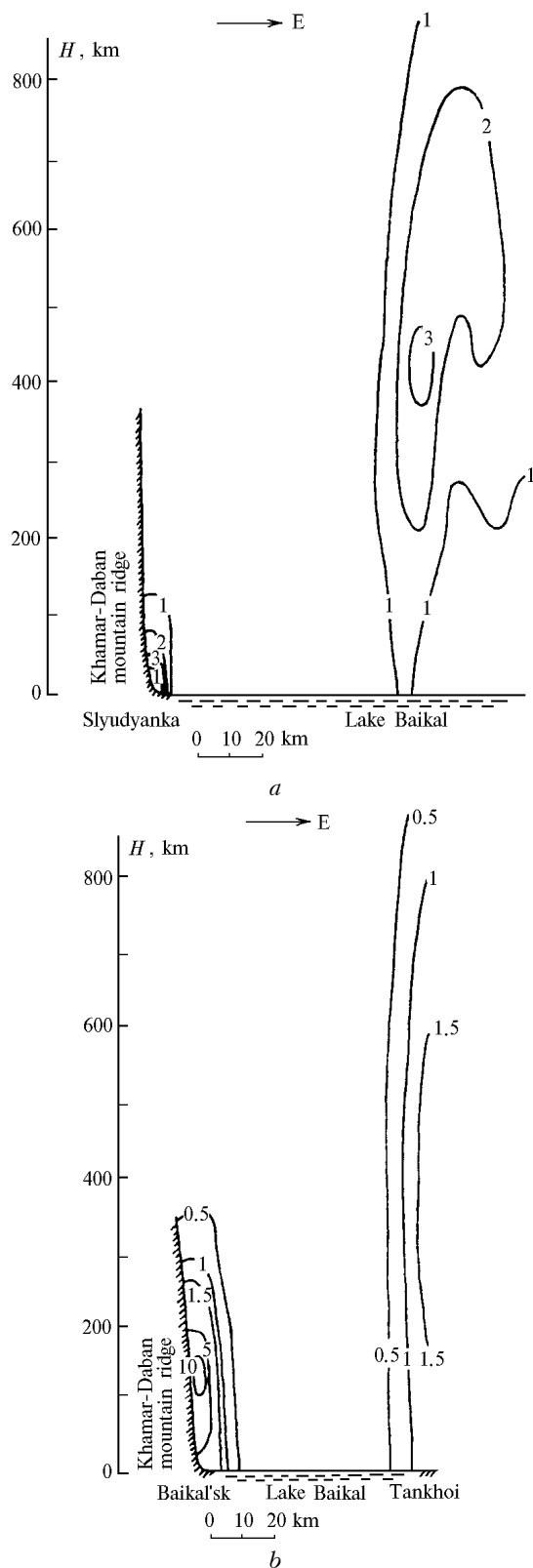


FIG. 2. Isolines of calculated nitrogen oxides concentrations,  $\mu\text{g}/\text{m}^3$ , in the cross sections Slyudyanka (a), Baikalsk-Tankhoi (b).

Figure 2 presents vertical cross sections in the direction from west to east. One of these passes through Slyudyanka while the other one through Baikalsk and Tankhoi. Here thin solid lines are isolines of the sum of nitrogen oxide and dioxide concentrations. The figure demonstrates their spread both from Slyudyanka and Baikalsk plants and Irkutsk-Cheremkhovo industrial region. The maximum concentrations of the oxides near Tankhoi ( $3 \mu\text{g}/\text{m}^3$ ), which are caused by the transfer along the Angara valley, are close to the corresponding concentrations over Slyudyanka ( $4 \mu\text{g}/\text{m}^3$ ). However, they are considerably lower than that over Baikalsk ( $10 \mu\text{g}/\text{m}^3$ ).

The results of calculations demonstrate that mountain ridges have a significant effect on the vertical distribution of pollutants in Southern Baikal region. The atmosphere pollution at heights above 400 m at north-west winds blowing at a speed no less than 10 m/s occurs mainly due to the effluents from Irkutsk-Cheremkhovo industrial region.

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