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ON ONE 3D NUMERICAL MODEL OF HARMFUL SUBSTANCES TRANSFER WITH ACCOUNT OF COMPOSITE OROGRAPHY

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Environment protection is one of the most urgent issues of today. So diagnosis, analysis of adverse substances and prognosis of their space-time distribution is one of the main problems of modern science. And numerical experiment, mathematical and computer simulation is an efficient method for analysis, diagnosis and prognosis of the factors causing ecological balance changes.

As know a harmful substance transfer throught the atmosphere can be described by the following equation [1-3]

$$\frac{\partial q}{\partial t}+u\frac{\partial q}{\partial x}+v\frac{\partial q}{\partial y}+w\frac{\partial q}{\partial z}=K_x\frac{\partial^2 q}{\partial x^2}+K_y\frac{\partial^2 q}{\partial y^2}+\frac{\partial}{\partial z}K_z\frac{\partial q}{\partial z}-aq+F, \tag{1}$$

where q is concentration; u,v,w are the axial components of wind velocity along axis OX, OY, and OZ; k_x, k_y, and k_z are the coefficients of turbolent diffusion; α - is the coefficient that determines the velocity of substance concentration changes during the process of substance decomposition and transformation; $F(x,y,z,t)$ is integral source.

Let the axis OX be directed along the earth parallel. The axis OY be directed along the meridian and the axis OZ be directed along the earth radius vertically upward.

Mountains exert a considerable influence on the atmosphere over a wide range of space and time scales [4]. Therefore for Caucasian region taking into consideration orographical effects in numerical weather forecast schemes has great importance. The sigma coordinate pressure normalized by its surface value its used as a way of conveniently incorporating variations in the height of the earth's surface. The governing equations for free baroclinic atmosphere, in the limits of quasi-statistic, is sigma coordinate system are the following [5.6]

$$\frac{\partial q}{\partial t}+u\frac{\partial q}{\partial x}+v\frac{\partial q}{\partial y}+\dot{\sigma}\frac{\partial q}{\partial c}=K_x\frac{\partial^2 q}{\partial x^2}+K_y\frac{\partial^2 q}{\partial y^2}+\frac{\partial}{\partial \sigma}\left(K_z\frac{\partial q}{\partial \sigma}\right)-aq+F, \tag{2}$$

$$\frac{\partial u}{\partial t}+u\frac{\partial u}{\partial x}+v\frac{\partial u}{\partial y}+\dot{\sigma}\frac{\partial u}{\partial c}-lv+\frac{\partial \Phi}{\partial x}-R\Theta\xi^{\frac{1}{k}}\sigma\frac{\partial \Pi_s}{\partial x}=0, \tag{3}$$

$$\frac{\partial v}{\partial t}+u\frac{\partial v}{\partial x}+v\frac{\partial v}{\partial y}+\dot{\sigma}\frac{\partial v}{\partial \sigma}-lv+\frac{\partial \Phi}{\partial x}-R\Theta\xi^{\frac{1}{k}}\sigma\frac{\partial \Pi_s}{\partial y}=0, \tag{4}$$

$$\frac{\partial \Pi_s}{\partial t}+\frac{\partial(u\Pi_s)}{\partial x}+\frac{\partial(v\Pi_s)}{\partial y}+\frac{\partial(\sigma\Pi_s)}{\partial \sigma}=0, \tag{5}$$

$$\frac{\partial \Phi}{\partial x} = -R\Theta\xi^{\frac{1}{k}}, \tag{6}$$

$$\frac{\partial \Theta}{\partial t} + u\frac{\partial \Theta}{\partial x} + v\frac{\partial \Theta}{\partial y} + \sigma\frac{\partial \Theta}{\partial \sigma} = 0, \tag{7}$$

where $\sigma = \frac{\xi - \xi_{top}}{\Pi_s}$, $\xi = \frac{P}{P_0}$ P is the pressure, $\xi = \frac{P}{P_0}$, $P_0 = 1000$ mb, $\Pi_0 = \xi_x - \xi_{top}$, $\xi_s = \frac{\Pi_x(x,y,t)}{\Pi_0}$, P_s is the pressure surface value, P_{top} =const, k=1,4 u and v are the wind velocity components in x ections, respectively, $\overset{0}{\sigma} = \frac{\partial \sigma}{\partial t}$, $\Theta-$ is the vertical velocity component, Θ is the potential temperature.

The system of equations (1)-(7) is solved in the area
$G = 0 \leq x \leq L,\ 0 \leq y \leq L,\ 0 \leq \sigma \leq l$
With bound Γ by the following initial and boundary conditions:

$$q|_{t=0} = q_0, \quad \Phi|_{t=0} = \Phi^0,\ P_s|_{t=0} = P_s^0,\ u|_{t=0} = u_g = -\frac{1}{l}\left(\frac{\partial \Phi^0}{\partial y} - A_1\frac{\partial \Pi_s^0}{\partial y}\right),$$

$$v|_{t=0} = v_g = -\frac{1}{l}\left(\frac{\partial \Phi^0}{\partial x} - A_1\frac{\partial \Pi_s^0}{\partial x}\right), \tag{8}$$

where $A_1 = R\Theta\xi^{\frac{1}{k}}\sigma$

At the top of the atmosphere we admit that the vertical velocity and vertical fluxes vanish,. At the bottom we assume air impenetrability through earth's surface. At

$$\sigma = 0 \text{ and } \sigma = l \text{ we have } \dot{\sigma} = 0, \frac{\partial q}{\partial \sigma} = 0. \tag{9}$$

Taking into consideration (5) and (9) we obtain for $\dot{\sigma}$

$$\dot{\sigma} = \frac{\sigma}{\Pi_s}\int_0^1 \left[\frac{\partial (u\Pi_s)}{\partial x} + \frac{\partial (v\Pi_s)}{\partial y}\right] d\sigma - \frac{1}{\Pi_s}\int_0^\sigma \left[\frac{\partial (u\Pi_s)}{\partial x} + \frac{\partial (v\Pi_s)}{\partial y}\right] d\dot{\sigma}. \tag{10}$$

Further rewrite equations (3), (4) for the two-dimensional case in the form

$$\frac{\partial u}{\partial t} + \frac{\partial E}{\partial x} + v\Omega = 0, \tag{11}$$

$$\frac{\partial u}{\partial t} + \frac{\partial E}{\partial x} + u\Omega = 0, \tag{12}$$

where $E = \frac{u^2+v^2}{2} + \Phi + A_t \ln \Pi_s, \qquad \Omega = \frac{\partial V}{\partial x} - \frac{\partial u}{\partial y}$.

At the lateral bounds in case of air inflow we set normal velocity component u or (v) and Ω. We obtain the other wind velocity component from (11) and (12)

$$\frac{\partial v}{\partial t} = -\frac{\partial E}{\partial y} - u\Omega, \qquad \textit{or} \qquad \left(\frac{\partial v}{\partial t} = -\frac{\partial E}{\partial x} - v\Omega\right). \tag{13}$$

In case of air outflow we have

$$\frac{\partial v}{\partial x} = 0 \qquad or \qquad \frac{\partial v}{\partial y} = 0. \tag{14}$$

Geopotential and temperature in both cases are extrapolated from internal area with the following expressions;

$$\frac{\partial}{\partial x}\left(\Phi + \frac{u^2}{2}\right) = -\frac{\partial u}{\partial t} + v\left(l - \frac{\partial u}{\partial y}\right), \ or \ \frac{\partial}{\partial y}\left(\Phi + \frac{v^2}{2}\right) = -\frac{\partial v}{\partial t} + u\left(l - \frac{\partial v}{\partial y}\right), \tag{15}$$

$$\frac{\partial q}{\partial x} = \frac{\partial u}{\partial y} = 0, \ \frac{\partial \Theta}{\partial x} = -\frac{1}{u}\frac{\partial \Theta}{\partial t}, \ \ or; \ \left(\frac{\partial \Theta}{\partial y} = -\frac{1}{v}\frac{\partial \Theta}{\partial t}\right). \tag{16}$$

But the use of sigma coordinates has several problems. One of them is the presence in governing equation of terms which, over steeply sloping orography, are individually relatively large, but which cancel. Much attention has been devoted to achieving an accurate computation of the two terms which form the net pressure gradient in the horizontal momentum equation [3,7]. To get ride of this problem in this paper we use the fine mesh for the compound orographic region; horizontal average temperature in the pressure gradient Term; sigma coordinate with changed top bound for this region.

For the purpose to keep full energy of the system of equations (3)-(7) in numerical model at every step of time we redistribute potential temperature and apply pseudo-viscosity terms.

$$\frac{\Delta l^2}{2}\left|\frac{\partial \varphi}{\partial x}\right|\left(\frac{\partial^2 \varphi}{\partial x^2} + \frac{\partial^2 \varphi}{\partial x^2}\right) + \frac{\Delta \sigma^2 \partial^2 \varphi}{\Delta x^2 \partial \sigma^2},$$

where $\varphi = \{u, v, \Theta\}^T$, $\Delta l, \ \Delta\sigma$ are horizontal and vertical grid steps, respectively.

In the domain G consider a grid $\bar{g}_1 = \{x_i = i\Delta x, \ j_j = j\Delta y, \ \sigma = k\Delta\sigma, \ t_s = s\Delta t\}$ $i = \overline{1, N}, \ j = \overline{1, M}, \ s = 0, 1, 2, ...$, here Δx, Δy are horizontal grid steps in direction x and y respectively; $\Delta\sigma$ is the vertical step.

The system of equations (2)-(7) with the initial (8) and boundary conditions (9), (13)-(16) is resolved in $\bar{g}$ by the Lax-Wendroff method. The parameters of the task had the following values:

$\Delta x = \Delta y = 100km, \ \Delta\sigma = 0.25, \ P_{top} = 300mb, \ N = 22, \ M = 6.$

In this model coarse mesh grid covers the large region other a fine mesh grid $\bar{g}_2$ is located inside of $\bar{g}_1$ and entirely covers the Caucasian region. The grid sizes for these two meshes are in the ratio 2 to 1. Numerical experiments were carried out both one-directional between two grids (boundary conditions for the smaller region were taken from the solution of the larger domain) and two-directional additionally (the solutions obtained in the small domain were used during solving in the large domain). Solution of the task in $\bar{g}_2$ is carried out with the initial (8) and boundary conditions (9), (13) - (16) using solutions obtained in the larger domain. Linear interpolations in time and space are used whenever necessary. Local boundary smoothing is applied to all variable at the gridpoints next to the bound areas with the expression [8]

$$\varphi_{2,j}(smoothed) = \frac{1}{2}u^{2,j} + \frac{1}{4}\{u_{1,j} + u_{2,j}\}.$$

During performing each numerical experiments we tested the computational stability of the numerical model. The conservation of the full and kinetic energy and tendency of changing of meteorological elements in time is performed by the following expression:

$$|\overline{\varphi_t}| = \frac{q}{N\Delta t} \sum |\varphi_{i,s+\Delta t} - \varphi_{i,x}| \,, \tag{17}$$

where $\varphi = \{u, v, \Phi, \Theta\}^T$, N is a number of all points of the grids. Numerical experiments have shown that in case of employment of two-direction method between two grids behaviors of the expression (17) and kinetic energy were not realitic in initial 8 hours of forecasting. It was not observed during calculation with one-dimensional interaction between two grids. Our investigations have shown that distinction of orography detalization on the different grids was more exhibited while performing two-dimensional computations. Therefore we apply one-directional interaction between two grids at initial 8 hours of computation and after that we apply two-directional interaction, called by combined method.

As we can see from the results given by two-directional method are better than the results obtained by one-directional method. In this case on average improvement is about 5.18%. But the best results we obtained applying combine nested grid method. In this case an average improvement in comparison with two-directional method is about 8.4%. Hence we can deduce, that including the detailed orography in the numerical model improves the quality of forecast and applying of the combine nested grid method in short-term predication in the Caucasian region gives the best results.

Some numerical experiments connected with environmental pollution were carried out on the basis of the given model. They were mainly different from the task of the meteorological conditions and capasity of harmful substances ejection. Due to the numerical experiments the basic part of harmful substances have fallen down neigh bour hood of the Main Caucasus Range. The relief has caused significant change of the surface speed field. In the western part of the Main Caucasus Range a horizontal flow around mountain range has taken place.

Numerical calculations have shown that distribution of concentrations in the Caucasus region represents compound hydrodynamics process, which is depended on the wind velocity, on the turbulance, on the location of the sources, on the initial distribution of the harmful substance's concentration, temperature, geopotential fields and the form of relief.

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