Analysis of a parallel algorithm for forecasting the release of toxic particles into the atmosphere in industrialized regions

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Annotation

The existing methods of parallelizing the atmospheric dispersion model can be divided into two categories, one of which uses a parallel computing interface to rewrite the source code, and the other directly distributes the repetitive elements in the computing task. This paper proposes an improved method based on the latter approach.

Аннотация

Существующие методы распараллеливания модели дисперсии атмосферы можно разделить на две категории, одна из которых использует параллельный вычислительный интерфейс для переписывания исходного кода, а другая непосредственно распределяет повторяющиеся элементы в вычислительной задаче. В данной статье предлагается улучшенный метод, основанный на последнем подходе.

Key words: mathematical model, numerical algorithm, approximation, transport and diffusion, atmosphere, air pollutants, particles deposition velocity

Growing urgency of environmental issues has emerged considerable amount of theoretical and experimental studies on the process of atmospheric air pollutants dispersion over the last decades. It is well-known that the air quality is influenced by many factors that require consideration in analyzing and forecasting its conditions. Accordingly, such a requirement necessitates the use of methods mathematical modeling and state-of-art machine-computing techniques which in many cases are preferable by economic and environmental criteria. Contamination of the surface layer of the atmosphere and land surface, including the transfer and diffusion of pollutants, and their deposition and concentration - this is a very complex process that subjected to the influence of many factors, including geographical and weather and climatic conditions, which are specific to one or another of the region. Aerosols deposition is of particular interest in solving the problems of monitoring and forecasting the contaminants concentration in the atmospheric boundary layer (ABL). The removal of pollutants from ABL mainly occurs due to wet or dry deposition. Wet deposition is the transport (fall-out) of a certain number of particles from the atmosphere to the underlying surface along with precipitation. Dry deposition is a continuous process that largely depends on the physico mechanical properties of the particles and characteristics of turbulent flows. Dry deposition is mainly modeled using a single parameter – the deposition rate, which is indicated empirically or determined from the corresponding theoretical relationships. When particles are sufficiently dense and large, then the deposition occurs under the action of gravity, represented in terms of the deposition rate. It should also be noted that thrown into the atmosphere aerosol particles affect the processes of cloud and precipitation by changing the microstructure of cloud particles and solar radiation and heat transfer processes in the atmosphere, also the temperature conditions of Earth's climate system. According to climatologists, the impact of ejected particles to the Earth's atmosphere is that aerosols scatter and absorb solar and thermal radiation, altering the radioactive balance of the atmosphere and the underlying surface. Climatic influence of aerosols ejected into the atmosphere industrial facilities causes a change in the radioactive properties (absorption and reflectance) of clouds, and their life time in the atmosphere and change in the relative humidity, which leads to the destruction of

the cloud. The presence in the atmosphere spreading aerosol particles leads to a negative effect of radiation, i.e., cooling the Earth's surface.

Tirabassi and Moreira, using an analytical solution of the advection-diffusion equation [1]

$$u_n \frac{\partial c_n}{\partial x} = K_n \frac{\partial^2 c_n}{\partial z^2} + w_s \frac{\partial c_n}{\partial z} \quad z_n \le z \le z_{n+1}, \quad n = 1:N,$$

showed that the deposition rate changes the particle concentration along the entire length of the ABL. The modeling results showed that gravitational deposition could greatly affect the final concentration of harmful particles in the air and the maximum concentration near the ground. The authors considered particles sizes from 10 to 100 µm at varying heights of emission sources and under different conditions of atmospheric stability. The deposition rate was calculated according to the Stokes law, and the height of the ABL was taken to be 1000 m. The authors also showed the effect of particle sizes on the concentration spread near the ground depending on the conditions of atmospheric stability. Obtained numerical results claim that under conditions of unstable atmosphere for particles of a diameter less than 10 µm the gravitational component of the deposition rate can be neglected. The authors applied a stepwise approximation to the problem by discretization the height h into sub layers. The solution of the problem was obtained using the Laplace transform.

In order to study the process of transport and diffusion of aerosol particles in the atmosphere taking into account their deposition rate, let us consider the mathematical model described by multidimensional partial differential equations

$$\frac{\partial\theta(x,y,z,t)}{\partial t}+u\frac{\partial\theta(x,y,z,t)}{\partial x}+v\frac{\partial\theta(x,y,z,t)}{\partial y}+\left(w-w_g\right)\frac{\partial\theta(x,y,z,t)}{\partial z}+\sigma\theta(x,y,z,t)=$$

$$=\mu\left(\frac{\partial^2\theta(x,y,z,t)}{\partial x^2}+\frac{\partial^2\theta(x,y,z,t)}{\partial y^2}\right)+\frac{\partial}{\partial z}\left(\kappa(z)\frac{\partial\theta(x,y,z,t)}{\partial z}\right)+\delta(x,y,z)Q; \qquad (1)$$

$$\frac{dw_g}{dt}=\frac{mg-6\pi krw_g-0{,}5c\rho sw_g^2}{m}$$

with appropriate initial

$$\theta(x,y,z,t)\big|_{t=0}=\theta_0(x,y,z);\; w_g(0)\big|_{t=0}=w_{g,0}(0) \qquad (2)$$

and boundary conditions

$$-\mu\frac{\partial\theta(x,y,z,t)}{\partial x}\bigg|_{x=0}=\xi\left(\theta_E-\theta(0,y,z,t)\right);\;\mu\frac{\partial\theta(x,y,z,t)}{\partial x}\bigg|_{x=L_x}=\xi\left(\theta_E-\theta(L_x,y,z,t)\right); \qquad (3)$$

$$-\mu\frac{\partial\theta(x,y,z,t)}{\partial y}\bigg|_{y=0}=\xi\left(\theta_E-\theta(x,0,z,t)\right);\;\mu\frac{\partial\theta(x,y,z,t)}{\partial y}\bigg|_{y=L_y}=\xi\left(\theta_E-\theta(x,L_y,z,t)\right); \qquad (4)$$

$$-\kappa(z)\frac{\partial\theta(x,y,z,t)}{\partial z}\bigg|_{z=0}=\left(\beta\theta(x,y,0,t)-f(x,y)\right);\;\kappa(z)\frac{\partial\theta(x,y,z,t)}{\partial z}\bigg|_{z=H}=\xi\left(\theta_E-\theta(x,y,H,t)\right). \qquad (5)$$

Here, θ – concentration of harmful substances in the atmosphere; θ0 – primary concentration; θE – concentration incoming through boundaries of considered area; x, y, z – coordinate system; u,v,w – wind velocity in three directions; wg – particles deposition rate; σ – atmospheric absorption coefficient; , μκ (z) – respectively, the diffusion and turbulence coefficients; Q – the emitter power; δi,j – Dirac function; f (xy) – entrainment of particles into the atmosphere from the underlying ground surface; β – particle-surface interaction coefficient; c – dimensionless value equal to 0.5; ρ – atmospheric density; r – particle radius; s – particle cross-sectional area; g – acceleration of gravity; ξ – dimensionality reduction parameter; , Lx,Ly– respectively, the length and the width of considered area; H – the height of the ABL

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