Simulating the dispersal of atmospheric admixtures in application to town-planning decision-making

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The model of the atmospheric admixture dispersal, in which the fields of wind velocity, temperature, and air humidity are determined using a closed system of the Navier–Stokes equations, is considered. The problem on determining the pollution of an anticipated residential microdistrict in the Ob town by car exhausts coming from Novosibirsk–Tolmachevo highway under construction is considered as a practical example. The performed series of calculations has enabled choosing an optimal town-planning decision to minimize the impact of car exhausts on the ecological situation in the microdistrict.

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The State Research Center of Virology and Biotechnology "Vector" has gained many-year experience in mathematical simulation of admixture dispersal in the atmosphere. For solution of "direct" problems, when the task is to find concentration fields from the known characteristics of sources, we use the approaches based on the semi-empirical equation of turbulent diffusion.¹ In the general case, to solve such a problem, one have to specify the wind velocity, temperature, and humidity fields, as well as the components of the tensor of turbulent diffusion coefficients. To calculate the admixture dispersal over relatively plain areas, we successfully use the method.² numerical-analytical In this case. determination of the wind velocity, temperature, and humidity fields is reduced to calculations by analytical equations specified in quadratures. The components of the tensor of turbulent diffusion coefficients are determined in accordance with the hypothesis on their proportionality to the corresponding components of the Reynolds viscous stress tensor, which we have experimentally justified earlier under the field conditions.³ These are determined by the model of an algebraic type.^{4,5}

The approaches developed were used, for example, to study regularities of atmospheric admixture dispersal over extended urban territories.^{6,7} the general In case. relief characteristics (buildings, blocks, parklands, water bodies, etc.) were taken into account through specifying the corresponding surface roughness parameters. For solution of a wide range of applied ecological problems, it is necessary to consider the spread of atmospheric admixtures over a crosscountry with more detailed consideration of various relief elements, for example, to perform computer simulation of admixture spreading with resolution at the level of individual buildings.

This paper presents a model for description of atmospheric admixture dispersal, in which the wind velocity, temperature, and humidity fields are determined using the closed system of Navier-Stokes equations that allows one to achieve higher spatial resolution than in the methods, we used earlier. As a practical example, we consider the problem on determination of the contamination of an anticipated residential microdistrict of the Ob town by car exhausts coming from the Novosibirsk-Tolmachevo highway under construction. The calculations performed have allowed us to choose an optimal town-planning, minimizing the impact of car exhausts on the ecological situation within the analyzed microdistrict.

Consider the mathematical formulation of the problem and the equations involved. The model is based on the system of nonstationary equations of continuous medium dynamics in stresses, as well as heat, humidity, and pollution transfer equations^{8–11}:

$$\begin{split} \frac{Du_1}{Dt} &= -\frac{1}{\rho} \frac{\partial p}{\partial x_1} + \frac{\partial \tau_{11}}{\partial x_1} + \frac{\partial \tau_{12}}{\partial x_2} + \frac{\partial \tau_{13}}{\partial x_3}, \\ \frac{Du_2}{Dt} &= -\frac{1}{\rho} \frac{\partial p}{\partial x_2} + \frac{\partial \tau_{21}}{\partial x_1} + \frac{\partial \tau_{22}}{\partial x_2} + \frac{\partial \tau_{23}}{\partial x_3}, \\ \frac{Du_3}{Dt} &= -\frac{1}{\rho} \frac{\partial p}{\partial x_3} + \frac{\partial \tau_{31}}{\partial x_1} + \frac{\partial \tau_{32}}{\partial x_2} + \frac{\partial \tau_{33}}{\partial x_3} + \lambda \vartheta, \\ \frac{D\vartheta}{Dt} &= \frac{L}{c_p} \Phi + \frac{\partial H_1}{\partial x_1} + \frac{\partial H_2}{\partial x_2} + \frac{\partial H_3}{\partial x_3} + J_\vartheta, \\ \frac{Dq}{Dt} &= -\Phi + \frac{\partial P_1}{\partial x_1} + \frac{\partial P_2}{\partial x_2} + \frac{\partial P_3}{\partial x_3} + J_q, \\ \frac{Dc}{Dt} &= \frac{\partial C_1}{\partial x_1} + \frac{\partial C_2}{\partial x_2} + \frac{\partial C_3}{\partial x_3} + J_c, \end{split}$$

$$\frac{\partial u_1}{\partial x_1} + \frac{\partial u_2}{\partial x_2} + \frac{\partial u_3}{\partial x_3} = 0,$$
$$\frac{D}{Dt} = \frac{\partial}{\partial t} + u_i \frac{\partial}{\partial x_i}.$$

In connection with the development of efficient methods for solving the equations of motion of a viscous liquid and because powerful computers are now available, it became possible to perform direct numerical simulation of turbulent motions. As was noted in Ref. 11, models of closure of small-scale motions have been intensely developed in recent years.

In such an approach founded by Deardorff,⁹ turbulence transfer processes are averaged starting only with the motion scale, which is not explicitly resolved at numerical approximation of the equations, while larger scales are calculated directly. Small treated here scales are through statistical approximation in the process of detailed consideration of large scales. The effect of unresolved small scales on the resolved large scales is characterized the turbulent using viscosity coefficients including semi-empirical constants. The Smagorinsky's approach⁸ turned out to be most popular among such approaches. Following Refs. 8-11, we represent the stress tensor τ_{ij} as a function of the deformation tensor D_{ii} of the mean motion in the following form:

$$\begin{aligned} \tau_{ij} &= k_m D_{ij}; \quad D_{ij} = \frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i}; \quad H_i = k_H \delta_{ij} \frac{\partial \vartheta}{\partial x_j}; \\ P_i &= k_H \delta_{ij} \frac{\partial q}{\partial x_j}; \quad C_i = k_H \delta_{ij} \frac{\partial c}{\partial x_j}; \\ k_m &= \begin{cases} \left(k_0 \overline{\Delta}\right)^2 |\operatorname{Def}|, \ \operatorname{Ri} > 1\\ \left(k_0 \overline{\Delta}\right)^2 |\operatorname{Def}| (1 - \operatorname{Ri})^{1/2}, \ \operatorname{Ri} \le 1; \end{cases}; \quad \frac{k_H}{k_m} = 3; \\ \operatorname{Def}^2 &= \frac{1}{2} \left(D_{11}^2 + D_{22}^2 + D_{33}^2\right) + D_{12}^2 + D_{13}^2 + D_{23}^2; \end{aligned}$$

 $\overline{\Delta} = (\Delta x \, \Delta y \, \Delta z)^{1/3}$ is the cell volume of a difference model; $k_0 = 0.21$; Ri = $\lambda \frac{\partial \vartheta}{\partial z} / \text{Def}^2$ is the Richardson number; λ is the convection parameter;

$$\begin{split} \Phi &= \begin{cases} \frac{c_p}{L} & (\gamma_a - \gamma_b), \ q \ge q_n \\ 0, \ q < q_n \end{cases}; \quad q_n = 0.622 \quad \frac{E(\vartheta)}{p} ; \\ E(\vartheta) &= 6.11 \cdot 10^{\frac{7.63(\vartheta - 273.2)}{\vartheta - 248.3}}; \\ \gamma_b &= \gamma_a \frac{p + 0.622LE/(AR\vartheta)}{p + 0.622L^2E/(c_pAR\vartheta^2)}; \\ A &= (c_p - c_v)/R; \ \gamma_a = Ag/C_p, \end{cases}$$

where x_i , $i = \overline{1, 3}$ are Cartesian coordinates; x_3 is the vertical coordinate; u_i are wind velocity components;

t is time; *p* is pressure; ρ is air density; J_{ϑ} , J_q , and J_c are the terms accounting for heat, humidity, and admixture sources; δ_{ij} is the Kronecker delta; Φ is the rate of formation of the liquid phase; q_n is the saturating specific humidity; $E(\vartheta)$ is the saturating water vapor pressure; γ_a is the dry adiabatic gradient; γ_b is the moist adiabatic gradient; c_p is the specific heat of air at constant pressure; c_v is the specific heat of air at constant volume; *g* is the acceleration due to gravity; *R* is the absolute gas constant; *L* is the latent heat of concentration (sublimation).

The boundary conditions for the above system of equations are formulated as follows. On solid surfaces:

- for components of the medium velocity, the non-penetration condition $u_n = 0$ is formulated in the direction normal to the surface, and the adhesion condition $u_{\tau} = 0$ is taken for the tangent direction, where u_n and u_{τ} are the normal and tangent components of the medium velocity, respectively;

- for the scalar parameters
$$\vartheta = \vartheta_n$$
 or $k_H \frac{\partial \vartheta}{\partial n} = \tau_\vartheta$,

 $\frac{\partial q}{\partial n} = \frac{\partial C}{\partial n} = 0$, where ϑ_n is the surface temperature, τ_{ϑ} is the heat flux.

At the entrance of the flow into the computational domain:

$$u_n = u_{in}, \ \frac{\partial u_{\tau}}{\partial n} = 0, \ \vartheta = \vartheta_{in}, \ q = q_{in}, \ C = C_{in}.$$

At the exit of the flow from the computational domain:

$$\frac{\partial u_n}{\partial n} = 0, \quad \frac{\partial u_\tau}{\partial n} = 0, \quad \frac{\partial \vartheta}{\partial n} = \frac{\partial q}{\partial n} = \frac{\partial C}{\partial n} = 0.$$

The system of equations is solved by splitting physical processes and spatial variables by use of the method of fictitious areas.^{10–12} The method of solution was tested using the classical test examples of motion of a viscous incompressible liquid: motion in two- and three-dimensional cavities, the problem of three-dimensional return current behind a bench, the problem of stationary convective motion between parallel isothermal plane heated up to different temperature, problem of motion under the effect of a turbulent thermal plume in the stratified medium,^{13–16} etc. The calculations were performed, in particular, on a system of densening grids, and some results obtained are considered in Ref. 17.

Consider an example of using the model for optimal town planning. The Novosibirsk— Tolmachevo highway that is under construction now passes through the Ob town and additionally divides its residential area. Therefore, the town should be protected against harmful pollution caused by car exhausts. The ecological situation is most adverse to the north of the highway in already existing microdistricts and blocks lying on the lee side from the highway with the prevailing southwestern winds in this region.

First, design organizations working on this project proposed to decrease the pollution of roadside territories by building a protective shield, which is now often used in town-planning practice. According to the designers' estimates, a 5-m high shield almost eliminates the harmful impact on the town territory and keeps the need to remove only seven private houses, falling in the pollution zone with the concentration of car exhausts in excess over the maximum permissible concentration (MPC). Taking into account that construction of the Novosibirsk-Tolmachevo highway is very important for the Ob town, which will get the shortest way to the regional center, and for further development of Tolmachevo International Airport, the territory of the northern part of the Ob town acquires a particular values.

At the same time, the presence of a protective shield all over the residential area will have the negative psychological and visual effect on people and will create unfavorable situation due to disconnection between the southern and northern parts of the town. Therefore, the design organizations were charged with finding alternative versions of protecting the residential area of Ob town. We have carried out the corresponding calculations using the model described above. For the calculations, we took the most adverse, almost calm, steady weather conditions. Note that with the allowance made for the wind rose such conditions are observed in the Ob town in 5% of cases

As the initial data on the intensity of emissions of most harmful compounds, we took the materials on nitrogen dioxide and sulfur dioxide emissions prepared by the Ekoniiproekt Company.¹⁸ The difference grid was $200 \times 100 \times 40$ with the horizontal step of 4 m, the vertical step of 1.5 m, and the time increment selected in accordance with the Courant

condition.¹² Such a choice of the spatial resolution allows, on the one hand, rather realistic description of the microdistrict and, on the other hand, determines large, but still acceptable volume of computations.

The calculations were carried out in the following order: a plain area without buildings and protective shield; buildings according to the design developed by Novosibgrazhdanproekt without a protective shield; buildings according to the design developed by Novosibgrazhdanproekt with a protective shield.

The first calculation series confirmed the estimates of the Ekoniiproekt Company. In particular, it was shown that at the distance of 200 m from the highway the nitrogen dioxide concentration would be twice as large as MPC. The zone of 1 MPC begins at the distance of 750 m from the highway. The pollutant is concentrated at the level of 1.5 m above the ground. At the height of 15 m the nitrogen dioxide concentration does not exceed 0.5 MPC.

The second calculation series with allowance for buildings but without the protective shield showed the tendency toward decreasing of the pollution at the height of 1.5 m. The pollution zones decrease due to vertical redistribution of nitrogen dioxide. The values exceeding 2 MPC are observed only near buildings from the direction of the highway. Insignificant penetration of harmful (exceeding 1 MPC) pollutants inside the microdistrict occurs only in interbuilding and arch spaces of multistorey (9–12 stores) buildings staying along the highway. Significant penetration of pollutants in depth of the microdistrict is observed only in the area of low (2–3 stores) buildings and along the access railroad, where the concentrations achieve 1-2 MPC. Figure 1 depicts the nitrogen dioxide concentration at the height of 1.5 m calculated for this case.



Fig. 1. Nitrogen dioxide concentration fields in the case of highway without protective shield. Isolines *1*, *2*, and *3* correspond to the concentration of 0.5, 1, and 2 MPC.

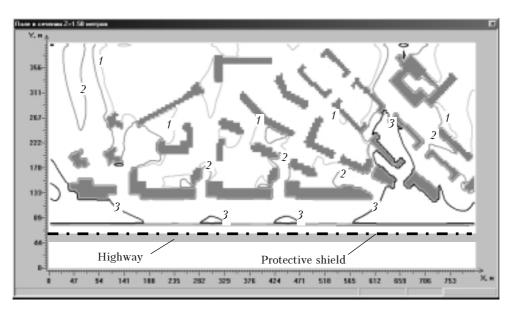


Fig. 2. Nitrogen dioxide concentration fields in the case of highway with protective shield. Isolines 1, 2, and 3 correspond to the concentration of 0.5, 1, and 2 MPC.

The third series of calculations carried out for the same microdistrict but with the protective shield showed that its presence does not change considerably the pollution pattern inside the microdistrict. Significant changes in the concentration field are observed only just near the shield itself (Fig. 2).

The results obtained and their analysis in cooperation with the specialists of Novosibgrazhdanproekt allowed us to conclude the following:

- The presence of multistory buildings forming a continuous barrier along the highway significantly changes the pollution pattern in the microdistrict and this allows the ecological situation to be improved through proper architecture decisions.

- Construction of a protective shield is economically inexpedient.

- The indoor air pollution in the buildings forming a shield along the highway can be decreased through the corresponding interior design by use of glass packs, installation of conditioners or forced ventilation, the use of ground-floor rooms for nonliving purposes (shops, offices, etc.). As a result, the municipal town-planning committee of the Ob town made a decision about inexpediency of constructing the protective shield in the zone of anticipated multistory building.

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