Numerical simulation of a two-component gas flow near a highway

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Abstract. Numerical simulation of the air flow near a highway was carried out taking into account injection of ethane through a system of low sources. Numerical model is based on full physical and mathematical models of continuum media and takes into account the phenomena of turbulent mixing of gas components in the surface boundary layer. Based on the calculation results, the fields of velocity distribution, turbulent parameters and impurity concentrations in characteristic sections near the road are obtained.

1. Introduction

One of the most important environmental criteria is the quality of the air, which contains pollutants in the gases and aerosols forms. Air pollutants, such as gaseous impurities of carbon dioxide, nitrogen oxides, sulfur dioxide, benzapyrene, aerosols with soot particles, heavy metal compounds, mineral and organic compounds are more of anthropogenic origin. According to [1], the main sources of emissions in the air of large cities are industry, transport, domestic fuel combustion and other anthropogenic sources. In contrast to industrial sources of emissions, the transfer of emissions from vehicles is local in nature near urban buildings and pedestrian zones and is characterized by a low spatial arrangement of sources relative to the level of the urban landscape. In pedestrian areas of densely built megalopolises, the composition of the air substantially depends on the quality of the transport infrastructure and the composition of the exhaust gases of vehicles.

Today, along with instruments for atmospheric monitoring and control over the level of emissions and aerosols in air, methods of mathematical and statistical analysis and methods of numerical modeling are actively used to describe and predict the parameters of transport, transformation and filtration of impurities in the lower atmosphere. An advantage of computational aerodynamics methods for solving such problems is ability to study nature of impurity transport phenomena and the influence of number of factors, such as the thermal regime of the boundary layer, turbulent mixing, filtration through buildings and green zones, on dynamics of the impurity on fairly detailed spatial scale. Thus, numerical modeling of the emission processes transfer in the surface layer of the atmosphere near the systems constructions and buildings is relevant both from the point of view of solving the fundamental problem of studying atmospheric processes, and from the point of view of solving the applied problem of predicting and improving air ecology.

Today there are a fairly large number of studies devoted to the numerical estimation of the processes of distribution and transfer of exhaust gases. In [2], a numerical simulation of air flow in the...
downtown of Melbourne city was performed to determine model constants and parameters of the turbulence model and further simplify the numerical model while maintaining sufficient calculation accuracy. In [3], a review of experimental work in wind tunnels aimed at studying air flows in urban areas and a description of the structure of flows and recirculation zones behind poor-flowing bodies, dangerous from the point of view of accumulation of heavy exhaust gases, is given. Detailed review of existing numerical models and schemes used to describe flows in urban canyons is given in [4].

Speaking about the numerical modeling of the processes of transporting exhaust gases, one of the most interesting works is the study [5], which analyzes the structure of the air flow taking into account the emission of exhaust gases near highways taking into account noise-suppressing barriers. The work [5] was carried out in accordance with experimental data on the estimation of flow parameters near a section corresponding to a part of the highway under conditions of a different location of this roadway relative to the main height level of the building [6]. The use of parametric models for setting the emission of exhaust gases from highways is presented in [7]. In [8, 9], the application of the RLINE model is described, which makes it possible to estimate the dispersion of pollutants from mobile sources. The authors' works [10–11] are devoted to the study of the aerodynamics of microdistricts of complex architecture and to the study of the influence of the thermal stratification of the boundary layer on the turbulent impurity transfer parameters.

2. Physical and numerical model

In this paper, we consider a model problem for studying the flow of multicomponent gas near a section of a highway. The statement of the problem corresponds to the experimental data [6]. To account for turbulent effects in the flow, we considered the Reynolds averaged Navier-Stokes equations for a two-component medium, supplemented by a $k$-$\omega$ SST turbulence model. The geometry of the computational domain is shown in Fig. 1 (a, b). The computational domain measures 140 cm wide by 245 cm length and 40 cm height (Fig. 1a). The substrate with neutral gas emission holes measures 24 cm wide and 24 cm long (Fig. 1b). To discretize the computational area, mesh of finite volumes based on tetrahedrons is constructed.

The air flow goes to the calculation area as shown in Fig. 1 (a). The profiles of the boundary conditions at the entrance to the computational area are constructed taking into account the vertical gradients of the gas-dynamic parameters. The vertical distribution of average velocity is described by a logarithmic profile [6]:

$$\frac{U}{u_*} = \frac{1}{k} \ln \left( \frac{z + d}{z_0} \right),$$

where $k=0.4$ – the von Karman constant, $u_* = 0.3$ m/s – reference velocity, $d=0.006$ m, $z_0=0.0052$ m.

As injection gas is taken ethane ($\text{C}_2\text{H}_6$) that is used in [6] to model exhaust gases. In experimental study [6] ethane is used because with a molecular weight of 30 is only slightly heavier than air and may be regarded as neutrally buoyant Ethane is injected through circular inlets arranged linearly in accordance with Fig. 1 (b). The total rate of gas at the outlet of the injectors is 1500 cm$^3$/min.

A symmetry condition was established along the lateral faces of the computational domain and a soft boundary condition for static pressure was set at the outer boundaries of the computational domain.

The calculations were carried out with the second order of approximation in space. The goal was to establish the flow field in the considered computational domain. As a solver, the software ANSYS Fluent was used.
3. Preliminary results

Based on the calculation results, the fields of velocity distribution, turbulent parameters and impurity concentrations in characteristic sections near the road are obtained. In fig. 2 shows the velocity vectors field over the substrate in a characteristic longitudinal section $Y_1$. Near the simulated highway, a compression of the flow is observed, that can be explained as interaction of the flow with the obstacle (Fig. 3). Formation of stagnant recirculation zones in the area between the rows of cars is observed.

![Figure 2](image-url)
Figure 3. Flow lines near a road fragment in plan.

Figure 4 shows the field of the mass fraction of ethane $C$ in a characteristic longitudinal section $Y1$. It can be seen from the figure that high concentrations of ethane are observed in recirculated stagnant zones behind bluff bodies. The transfer of impurities behind a system of bluff bodies has a highly spatial character.

![Image of flow lines](image1)

Figure 4. Field of mass fraction of ethane $C$ in a characteristic vertical section $Y1$.

4. Conclusions
A numerical simulation of the air flow near the highway was carried out taking into account the injection of ethane through a system of low sources. Based on the calculation results, the distribution fields of velocity vectors, turbulent parameters and impurity concentrations in characteristic sections near the highway are obtained and the flow structure behind the system of poorly streamlined bodies is described. In further work, it is planned to clarify the parameters of the problem and conduct a quantitative comparison of the results with experimental data [6].

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