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Numerical modeling of pollutant transport in the atmospheric boundary layer using ANSYS

Abstract. The purpose of research is to simulate the dynamics of wind velocity distribution, impurities in the atmospheric boundary layer using ANSYS software system. Computational modeling is a basis for successful environmental problems researches, in particular, to predict the spread of polluting substances, hazardous gas clouds and impurities in the air from man-made sources and optimization the financial costs of environmental measures. The solution of such problems requires the achievement of the following objectives: the mathematical model creation of the atmospheric boundary layer dynamics, design scheme description, setting the boundary and initial conditions, the process of problem solving, convergence solution control, the results processing and analyzing, what was done in this paper.

Key words: atmospheric boundary layer, numerical modeling, ANSYS software system, spread of polluting substances

Introduction

Pollution increases due to increasing anthropogenic stresses environmental, particularly in the atmosphere. Therefore, monitoring and forecasting of air pollution have always been and remain an important issue. The essence of the study is to model the dynamics of inhomogeneous turbulent flows of different substances occurring on the non-uniform earth's surface in the atmospheric boundary layer due to increased air contamination with dust and condensation products. The atmospheric boundary layer is the layer of air between 300-400 m. to 1-2 km. adjacent to the earth's surface. Turbulence is important in the boundary layer. In this regard, the properties of the boundary layer are mainly determined by thermal and dynamic effects of the underlying surface.

Examination of physical processes and phenomena in the layer of the atmosphere at 200-2000 meters thick, concerning the earth's surface has an essential scientific and practical significance. The structure of the layer affects on flora and fauna of the planet, on the populations life conditions greatly.

The regularity of physical processes occurring in the boundary layer and other atmospheric layers different in many ways. Status of the boundary layer is very closely linked to the state of the Earth surface. Meteorological values are subjected to

sudden changes in the atmospheric boundary layer with altitude and time. The vertical gradients of meteorological components are higher in the given layer than in the other layers [1].

Main body

To calculate the immense amount of researches and applications we need to find vertical profiles of meteorological elements and characteristics of the atmospheric boundary layer (ABL), characterizing the meteorological phenomena that occur in it, and even the processes of pollutants and aerosols transport. Solving horizontally inhomogeneous ABL problems is the most difficult process [2].

The most famous modern product is ANSYS software system, which is a multi-purpose software package for physical processes and phenomena numerical modeling.

ANSYS Workbench is software platform with extensive capabilities for integrating different applications into a single workspace and exchanging data between them. Workbench project is a virtual space which forms the calculating pattern using various combinations of modules [3].

Five tasks were solved in order to create a model of the atmospheric boundary layer dynamics in ANSYS Workbench:

- geometric model creation / import;

- computational domain spatial discretization (geometric area covering with finite element / finite volume grid);
- physics-mathematical model selection, design scheme description, setting the boundary and initial conditions;
- the process of problem solving, convergence solution control;
- the results processing and analyzing.

The first step in solving the problem was the creation of geometrical model in the Design Modeler module. The area of 6000 m (horizontal size) to 1500 m (vertical size) were chosen to set the atmospheric boundary layer geometry. Spatial sampling computational domain was made at the second stage, which corresponds initial geometric model obtained in the first step. Construction of grids was made by using Meshing module. Computational grid (dimension is 200 × 80) was built for the task. Grid built with pressed boundary layers near the solid boundary (land) using Sizing component. Mesh generation performed with Mapped Face Meshing method.

The third step of solving the problem is the right choice of necessary design module. ANSYS FLUENT module was used to obtain the solution of the nonstationary problem.

The ANSYS software complex pays special attention to the advanced turbulence models development for efficient and accurate calculation of turbulent processes. The calculation of the problem occurred on two-parameter k-ε turbulence model. Two differential equations for the turbulent kinetic energy transfer and the transfer of turbulence dissipation are solved in presented model. Enhanced Wall Functions was used in this model of turbulence. This method is obtained by combining linear (laminar) and logarithmic (turbulent) laws of the wall, using the function proposed by Kader [4].

An important step in calculation model preparation is the materials selection with specifying their physical properties in the Materials section of the project tree. Four materials were selected for the problem: air, nitrogen, oxygen, water-vapor. The percentage of each component in the air was found according to meteorological data in the boundary conditions of the problem.

In the paper the following boundary conditions were set at the entrance to the computational domain: Velocity Inlet condition. It is useful for specifying velocity and scalar parameters. Since wind speed varies with height, the input condition was for velocity was:

$$U(z) = U_0 \cdot \left(\frac{y}{H}\right)^\beta \tag{1}$$

where, U_0 is the wind flow average speed at height H , β is the coefficient depending on the terrain type. The temperature was set by temperature distribution according to the height. The temperature is lowered by 1°C for every 100 m. Such plot is described by the equation:

$$T(z) = T_0 - \gamma y \tag{2}$$

where T_0 is the temperature at the earth's surface; γ is the vertical gradient of temperature [5].

The boundary conditions on the wall:

- On-slip condition at the wall.
- The temperature of the wall is 15°C.

Pressure-Based solver setups were selected at the fourth stage. Pressure-Based solver connects the calculating algorithm for the Navier-Stokes equations, based on the pressure correction method. Initialization is performed using Solution Initialization window. By default, there is the hybrid method of initialization, in which the pressure and velocity fields are determined by solving the Laplace equation.

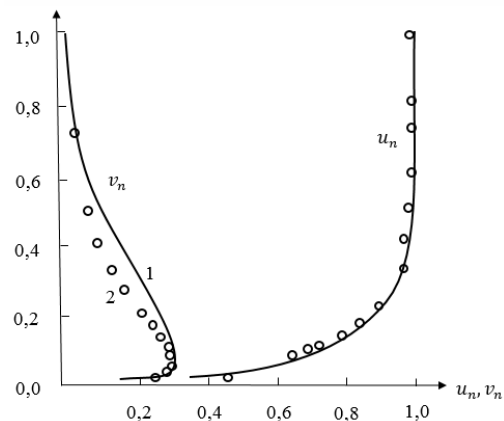


Figure 1 – Vertical profiles of wind speed with $U = 6.6$ m/s
1 – calculated profile, 2 – experimental points

The results of the atmospheric boundary layer dynamics calculations

Comparison of the numerical solution results with field profiles of the wind in the atmospheric boundary layer from measure were presented by Vager B.G. and Nadezhina E.D. [5]. Results of the study are presented in Figure 1, which shows that

for different values of the geostrophic wind u_n -component profile of the wind speed is almost the same as the experimental. However, between the calculated and experimental v_n -component profile there are differences in the middle part of the boundary layer.

Below there are the results of wind speed u, v – components numerical calculations in the PC ANSYS

The dynamics of the velocity components (u, v) (Fig. 2) is qualitatively consistent with the results from [5], (Fig. 1), which allows us to conclude that the assembled model in ANSYS is adequate.

Modern studies of large urban environment, as well as theoretical and applied environmental problems associated with them, have a considerable interest, as the city became a leading place of human habitation. Modeling of carbon dioxides dynamics will help to better understanding how CO_2 can accumulate and affect the Earth's atmosphere, and what methods can be taken for the planet conservation.

Figures 3, 4 show the distribution of CO_2 in the air from the emission source at different times, when the wind speed is 3 m/s (Figures 3) and 12 m/s (Figures 4).

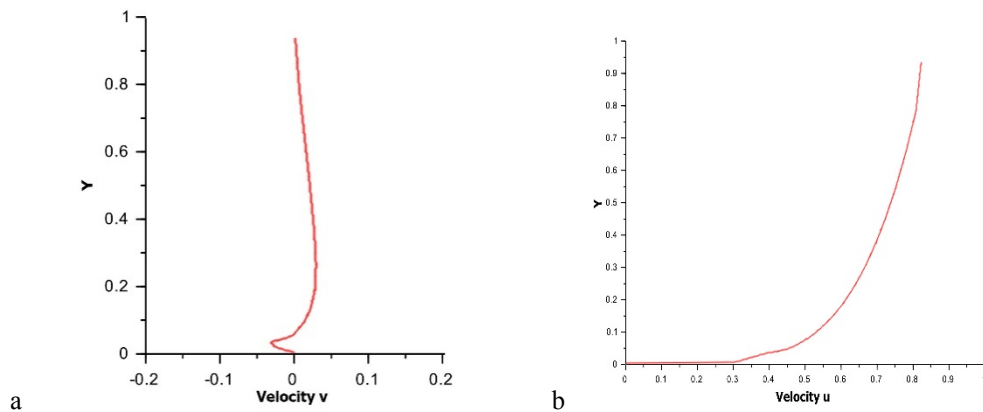


Figure 2 – Wind speed profile with $U_0=6.6$ m/s
a) u-component; b) v-component

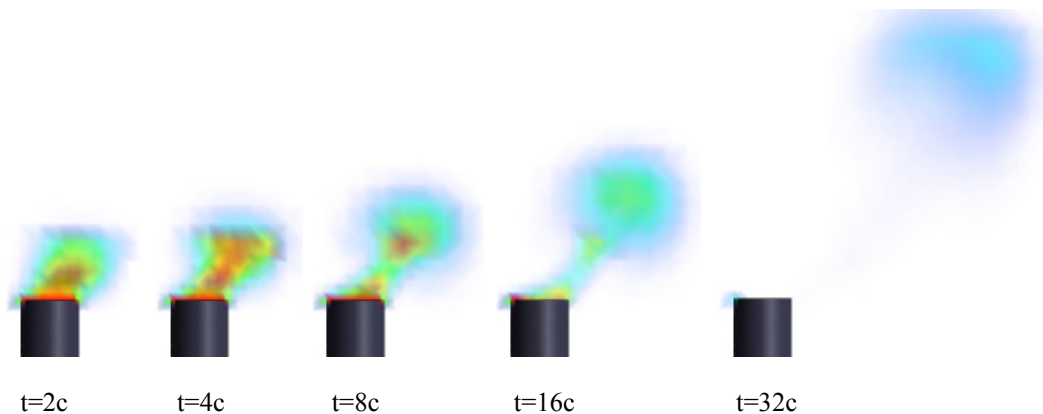


Figure 3 – Distribution of CO_2 in the air from the emission source at different times with wind speed 3 m/s

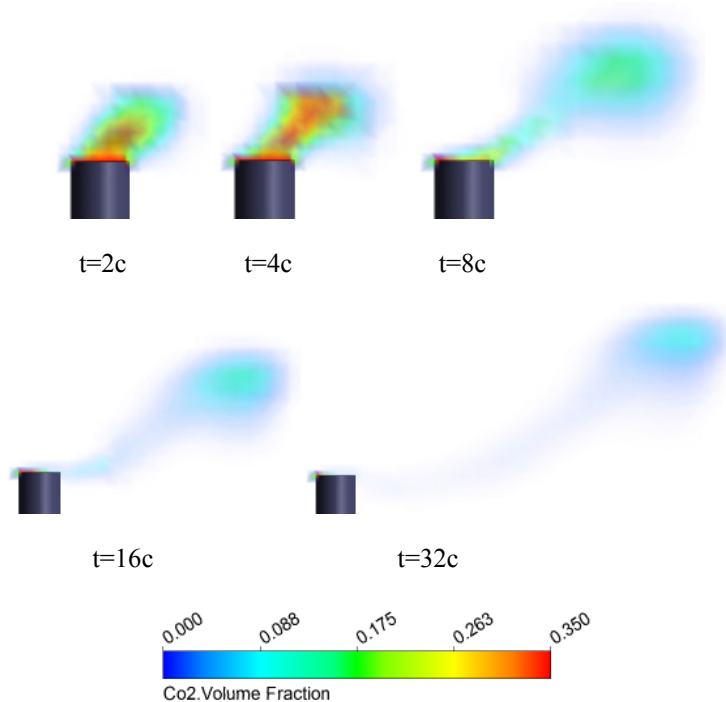


Figure 4 – Distribution of CO₂ in the air from the emission source at different times with wind speed 12 m/s

The initial condition was indication of CO₂ volume fraction – 0.350. According to Figure 3 CO₂ spread differs slightly (only at 230-250 m) after four seconds from the emission start with wind speed of 3 m/s and 12 m/s. The maximum concentration of CO₂ is observed near the source of emission. After 8 seconds there is the emergence of two foci with the highest concentrations: near the source of emission and less pronounced at the distance of 200 m with wind speed of 3 m/s and 250 m with 12 m/s horizontally. The emissions extend to a height of about 300 m in the vertical direction. Horizontal compiling increases with rising transfer duration of impurities, so by 32 seconds the highest concentration observed at a distance of 600 meters from the source at a wind speed of 3 m/s and 1200 m at 12 m/s. While the greatest concentration of the cloud is located at an altitude of 1000 m. Concentration becomes less with more impurities transfer.

Conclusion

Numerical experiments allow to solve problems environmental impact assessment of pollution spreading from man-made sources in the project stage with sufficient accuracy. Modern computational models for analyze and forecast the state of the surrounding environment will help to minimize

the environmental hazard degree, improve the comfort level of population accommodation and recreation and optimize the financial costs of environmental measures.

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