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S.D.Maussumbekova
Faculty of Mechanic- Mathematical, Al-Farabi Kazakh National University
saulemaussumbekova@gmail.com
K.Khan
Faculty of Mechanic- Mathematical, Al-Farabi Kazakh National University

COMPUTATIONAL STUDY OF TEMPERATURE STRATIFICATION EFFECT ON HARMFUL GASES EXPANSION IN THE ATMOSPHERE

Abstract

To date, the study of atmospheric pollution is of great interest. Assessment, monitoring and calculation of concentrations of harmful impurities in the atmosphere with their source is based on theoretical studies, and it is possible to make short-term forecasts used to control emissions from industrial enterprises. Disposal of waste by industrial enterprises, often consisting not only of light impurities, but also of heavy elements, does not always control what constitutes a danger to living creatures and flora in the affected area.

Computational model is constructed for determination of harmful impurities expansion in atmosphere, which is most serious environmental problems in many industrial cities in the world. Numerical calculations are obtained by programm complex ANSYS. There is given analysis and results of calculations determining the distribution of harmful impurities concentrations in different temperature gradient. Calculations are conducted for different pollutant-emission rate from point source. There is studied the influence of temperature in ground layer on the dynamics of harmful impurities concentration from point source. Obtained results allow to predict of distribution contour of impurities and its extent.

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

Introduction

Dispersion of pollution represents an important environmental problem with respect to human health. In urban areas, several sources of pollution (e.g. wind-blown dust, vehicle exhaust, toxic and odorous emissions) may be unpleasant and dangerous. Among them, pollutant emissions from rooftop stacks is a factor that can seriously affect the quality of fresh-air at intakes of the emitting and/or surrounding buildings, and potentially compromising the well-being of these buildings' occupants. Additionally, inside cities − where the building density increases − the stack emissions can be accumulated between buildings, thus inducing an increase of the contaminant concentration because reduced airflow passes through the zone's boundaries as compared to free-stream flow.

The problem of environmental protection and restoration is becoming one of the most important tasks of science, the development of which is stimulated by the ever-increasing pace of technological progress in all countries of the world. The rapid development of industry contributed to the emergence of an acute problem for humanity - the preservation of ecological systems that historically formed on our planet. In recent decades, environmental systems have experienced a significant impact of natural, especially anthropogenic factors, changing in an undesirable direction for nature. The increased concentration of pollutants is observed in the atmosphere of almost every industrial city, so there is a need to solve the problem of assessing and modeling the spread of pollutants in the atmosphere from local stationary sources to prevent or reduce their impact on the ecosystem. A wide range of environmental protection tasks is being solved using mathematical modeling methods. This approach allows testing multiple options for work, to predict various scenarios for the development of the process while varying the initial data. A lot of articles have been published in which studies of atmospheric pollution from different directions and taking into account various factors are presented [1-6].

Numerical simulations with CFD offer some advantages compared to other methods; they are relatively less expensive, they provide results of flow features at every point in space simultaneously [7]) and they do not suffer from potentially incompatible similarity because simulations can be conducted at full scale [8]. In addition, at the micro-scale, the CFD technique is the preferred way of investigation and very suitable for parametric studies for various physical flow and dispersion processes [9]. Due to the rapid development in computer hardware and numerical modelling, CFD has been increasingly used and adopted to simulate the flow development and pollutant dispersion [10]. Many studies have shown that the approach is capable of reproducing the qualitative features of airflow and pollutant distributions [11]. However, the accuracy and reliability of CFD are of concern, thus solution verification and validation studies are imperative [12]. Since experience has already shown that numerical results do not compare among themselves [13], experimental tests (i.e. field and reduced-scale measurements) appear unquestionably necessary for fulfilling the requirements of assessing the quality of CFD simulation [14]. In addition, one of the objectives of laboratory studies has frequently been to aid the development of dispersion algorithms that can be used in dispersion modelling packages to predict behaviour near and around buildings [15].

In this paper we consider the effect of temperature stratification on the distribution of concentrations of harmful substances in the atmosphere emitted by industrial enterprises through local sources (pipes). The mathematical model of the problem is a system of Navier-Stokes equations, energy equations and equations for the k-ε model of turbulence. This system of equations is solved with using of FLUENT package [17].

Physical statement of problem

One of the conditions affecting the dynamics of the distribution of harmful substances is the stratification of temperature in height, due to the ability of the earth's surface to absorb or radiate heat [1].

The paper deals with the problem of spreading the concentration of harmful substances in the atmosphere emitted by industrial enterprises through point sources (pipes), taking into account of temperatures variation with vertical. Computational domain is the rectangle with width - 60 m and height - 30 m. The point source (pipe) is located at 4 meters apart from left boundary. Diameter of source's mouth is 1.2 m, height of source is 7 m. Figure 1 schematically shows computational domain.

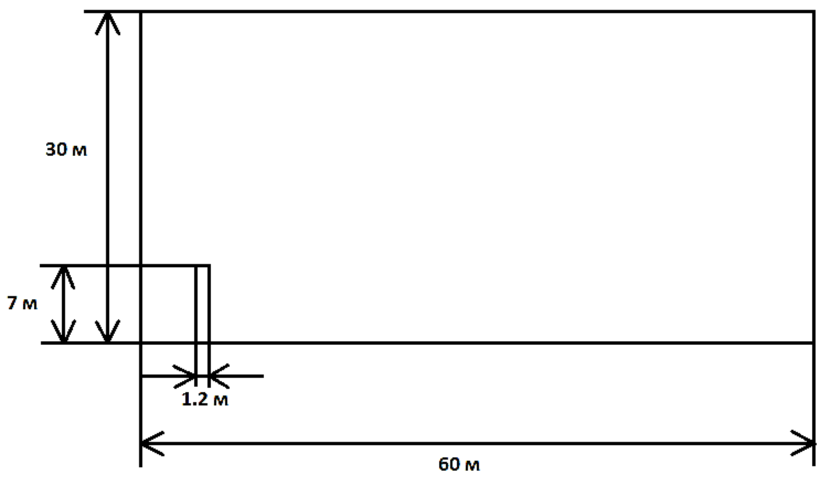


Figure 1. Scheme of computational domain.

Solution method

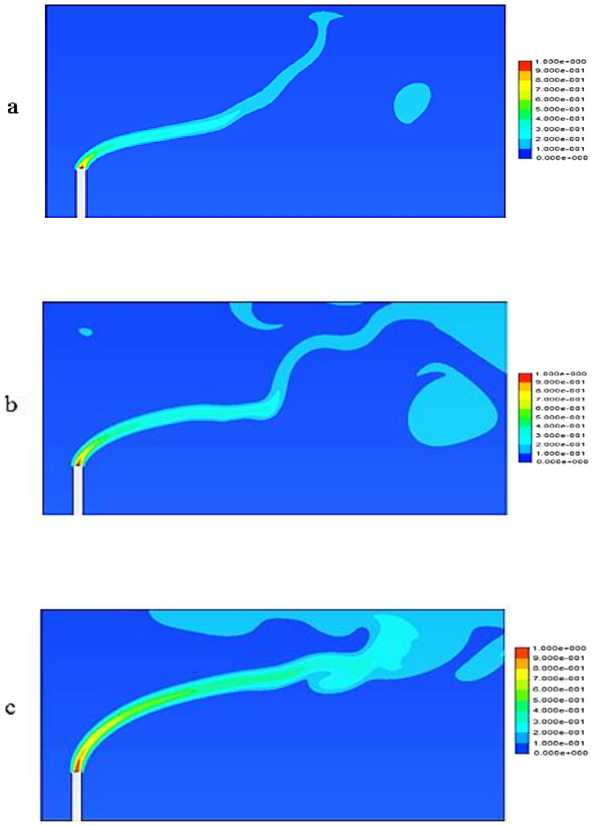
ANSYS software was used for solving of problem. At first stage, geometry of object was created with the help of built-in DesignModeler editor. Mesh editor allows sampling computational domain. Transition to Setup editor allows setting initial and boundary conditions of task, and choose solution method. In General we set Type - Pressure-Based, Time – Transient, VelocityFormulation – Absolute, 2DSpace – Planar. Below we put a tick in front of Gravity and assign value along vertical axis -9.8 m / s^2. In Models, we add energy equation, We change Viscous to Stardard k-ε, Species to SpeciesTransport, here we choose MixtureMaterial - methane-air, Reactions - Volumetric and Turbulense - Chemistry Interaction - Eddy-Dissipation. Here, we use UDF to set temperature gradient. We create *.c file, where we set temperature profile. To use it in the project, we call menu Define -> DefineFunctions -> Interprete ..., select created file. After that, in settings of Cell Zone Conditions, we put a tick in front of FixedValues and change Temperature from none to udf_y_temperature. Specifying values on boundaries of domain is done in Boundary Conditions tab. Values of incoming flow velocity to domain in air_inlet, emission rate of methane from pipe in gas_inlet are specified. Oxygen mass fraction in air_inlet is 0.23, and methane mass fraction in gas_inlet is 1. In air_inlet, temperature is changed from none to udf_y_temperature.

As solution method, the method SIMPLE (Semi-Implicit Method for Pressure Linked Equations) was chosen, put it otherwise - splitting method by physical parameters. Then calculation is initialized.

Analysis of results

Calculations were carried out in different variations of temperature gradient and rate of harmful impurities emission from mouth of source. Results were obtained at pollutant-emission rates: 2.5 m/s, 4 m/s, 10 m/s. Air flow from the left moves at velocity of 0.5 m/s. This airflow velocity according to the Beaufort scale corresponds to determination of wind strength - quiet [9]. That is, in this case, direction of wind can be seen through smoke, but not over weathervane, leaves of trees remain motionless. Presented figures determine the state of plume on the thirtieth second. Iteration step in time is 0.1 s.

Figure 2 shows methane (CH_4) concentration distribution in case of temperature decrease with altitude.



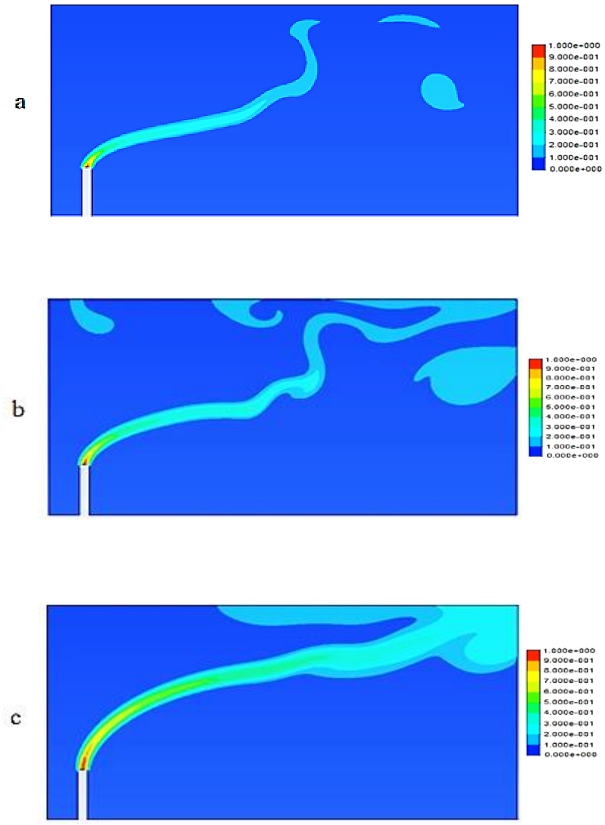


Figure 2. Methane (CH_4) concentration distribution in case of temperature decrease with altitude

Figure 3. Methane (CH_4) concentration distribution in the case of inversion (increase in temperature with altitude)

Figure 3 shows methane (CH_4) concentration distribution in case of inversion. In comparison with Figure 2, which presents the case of methane concentration distribution at negative temperature gradient, most of impurities is transported on considerable distance in direction of wind motion before it reaches considerable concentration in earth's surface. This is due to dominance of small-scale mechanical turbulence arising at low temperature gradients [9]. In comparison with figure 2, which presents the case of methane concentration distribution at positive temperature gradient, it can be seen that contaminants are removed over long distances, so low concentrations of harmful substances reach ground level and weak mechanical turbulence arises [7].

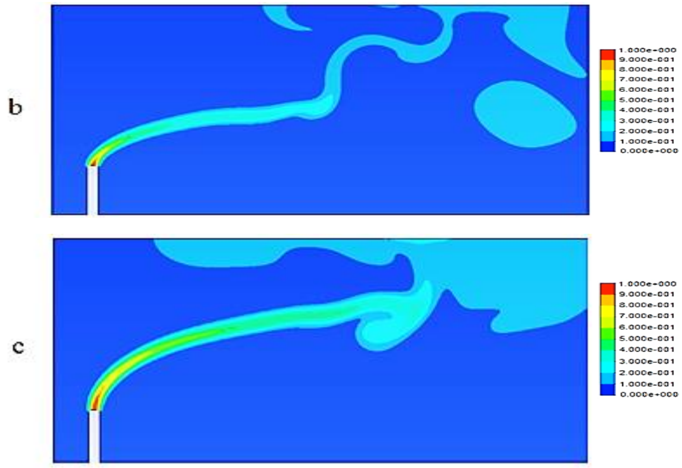


Figure 4. Methane (CH_4) concentration distribution in case when the source mouth is located above the upper boundary of inversion layer

Figure 4 is picture of methane concentration distribution emitted into atmosphere by point source, in case when the source mouth is located above the upper boundary of inversion layer.

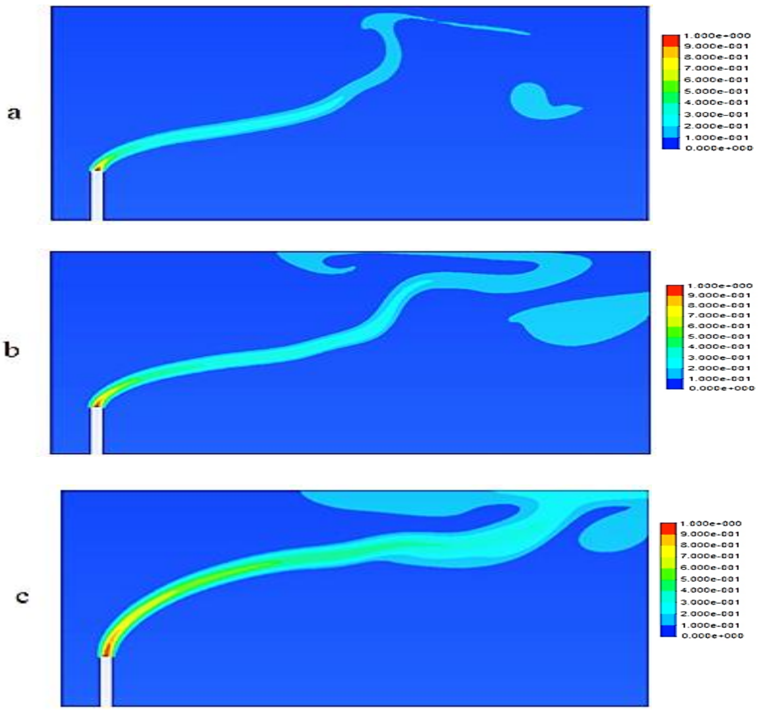


Figure 5. Methane (CH_4) concentration distribution in case when the source mouth is located below the lower boundary of inversion layer

Inversion layer, located below level of source mouth, is natural barrier to lowering pollutants to earth's surface. Figure 5. describe of methane concentration distribution which emitted into atmosphere by local source, in case when the source mouth is located below the lower boundary of inversion layer. It can be noted that significant parts of concentration are separated from source by considerable distance. Dispersion also occurs at considerable distance from source. This is due to the fact that above mouth of source is powerful inversion layer, which prevents dispersion of harmful substances released into the atmosphere. Significant concentrations of harmful substances remain closer to earth's surface. Inversion layer located above the level of source's mouth is obstacle to dispersion of harmful substances, and therefore impurities concentration in surface layer can be higher than calculated one in several times.

Figure 6. describes of methane concentration distribution at pollutant-emission rate of 2.5 m/s. Four cases are considered, each of which corresponds to given temperature gradient. 6 (a) is characteristic for the case when temperature decreases with altitude; 6 (b) - for the case of inversion; 6 (c) - for the case when mouth of source is located above the upper boundary of inversion layer; 6 (d) - for case when the source mouth is located below the lower boundary of inversion layer.

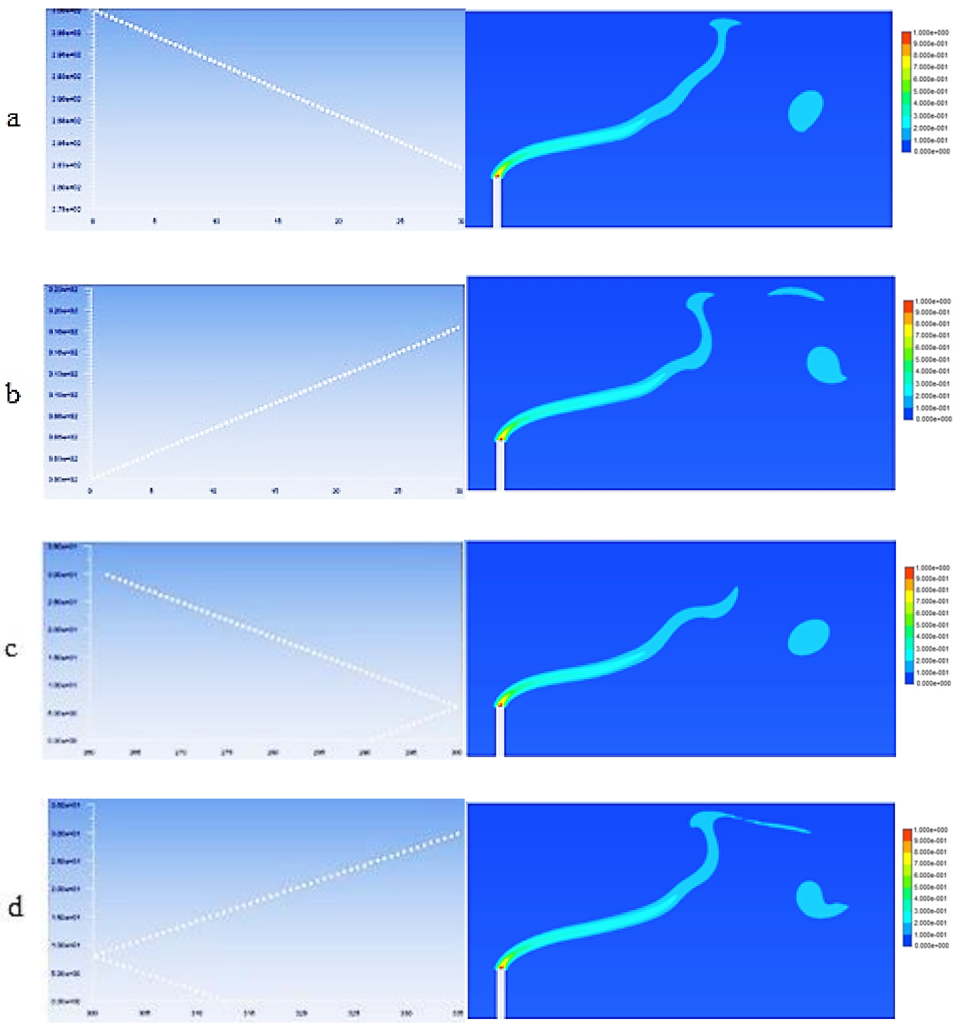


Figure 6. Methane (CH_4) concentration distribution for various initial temperature profiles in case when pollutant-emission rate is 2.5 m/s

In Figure 7 were presented the methane concentration distribution at pollutant-emission rate of 4 m/s. Four cases are considered, each of which corresponds to given temperature gradient. 7 (a) is characteristic for the case when temperature decreases with altitude; 7 (b) - for the case of inversion; 7 (c) - for the case when mouth of source is located above the upper boundary of inversion layer; 7 (d) - for case when the source mouth is located below the lower boundary of inversion layer.

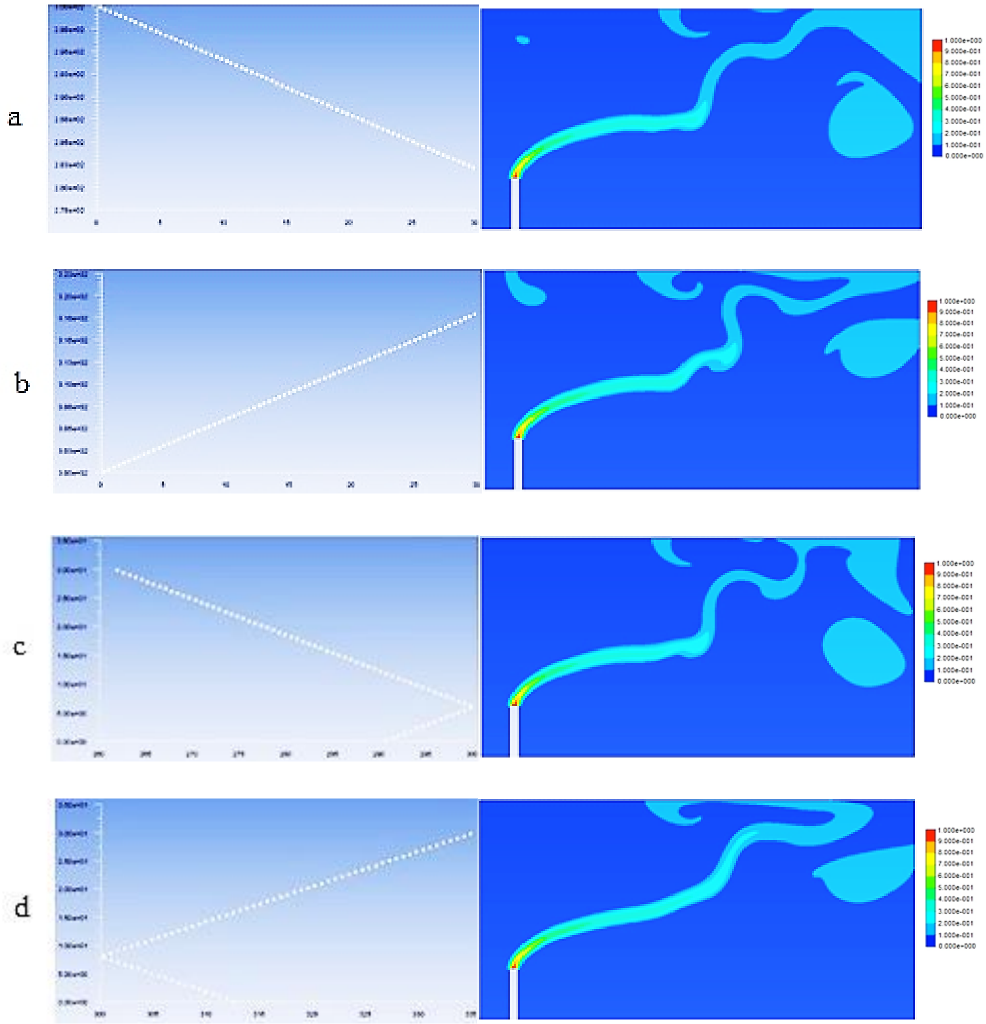
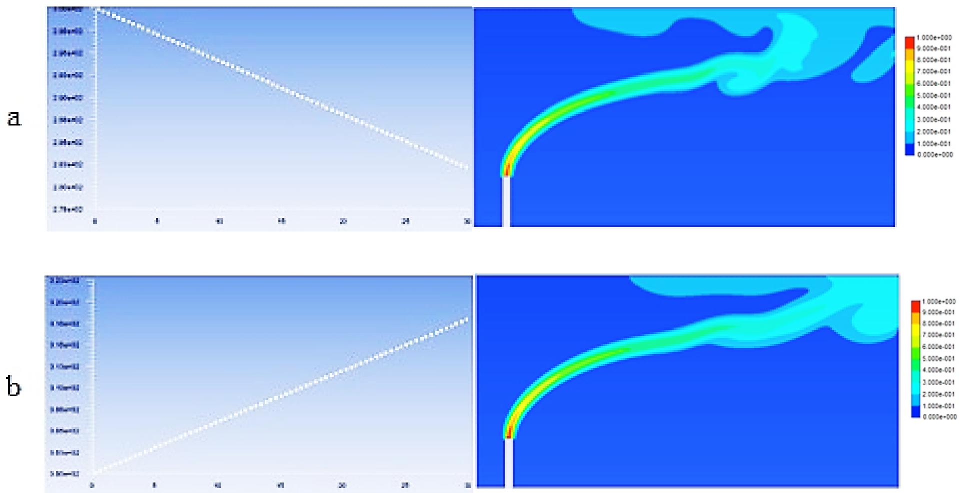


Figure 7. Methane (CH_4) concentration distribution for various initial temperature profiles in case when pollutant-emission rate is 4 m/s

The computational experiment was done for the speed 10 m/s. Four cases are considered, each of which corresponds to given temperature gradient. 8 (a) is characteristic for the case when temperature decreases with altitude; 8 (b) - for the case of inversion; 8 (c) - for the case when mouth of source is located above the upper boundary of inversion layer; 8 (d) - for the case when the source mouth is located below the lower boundary of inversion layer.



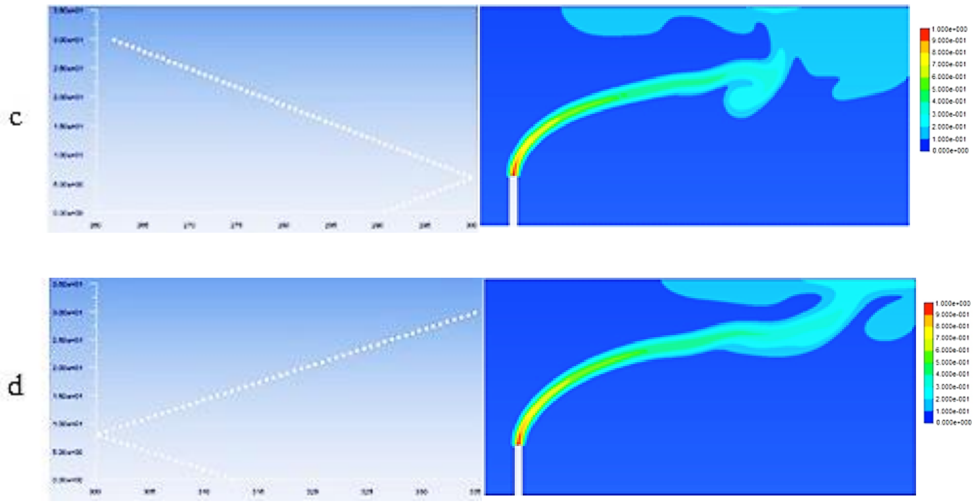


Figure 8. Methane (CH_4) concentration distribution for various initial temperature profiles in case when pollutant-emission rate is 4 m/s

Thus, represented results allow to note wind influence importance to harmful substances distribution in atmosphere which are thrown out by point source of industrial enterprise.

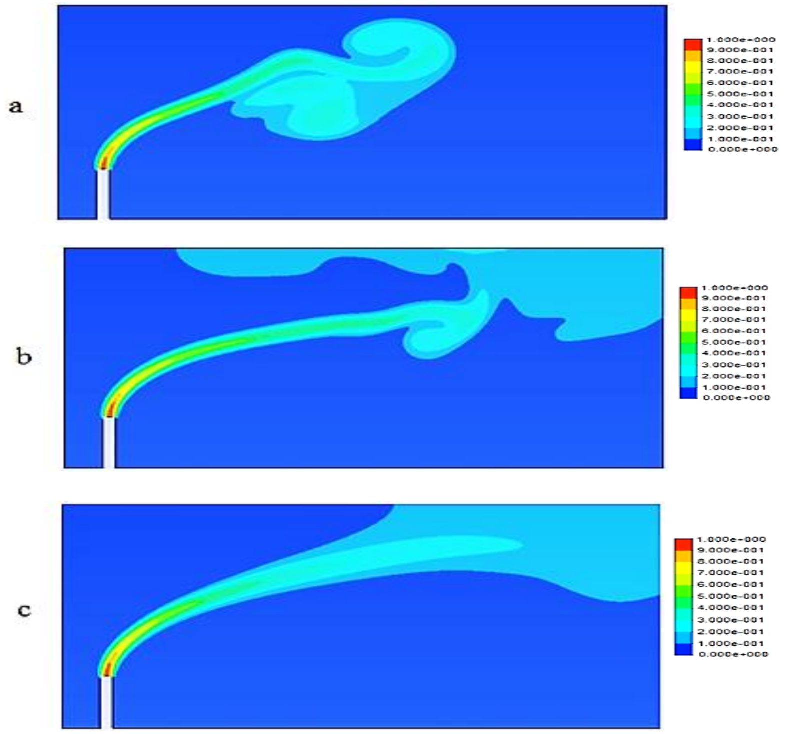


Figure 9. Temporal distribution of methane (CH_4) concentration in case when the upper boundary of inversion is located below mouth of source

Figure 9 corresponds to methane concentration distribution of at t = 10 sec (10 (a)), t = 30 sec (10 (b)), t = 60 sec (10 (c)). As can be seen, at first stage, significant concentrations remain near mouth of source, scattering is noticeably observed. In second stage, significant concentrations are transfered to more remote distance from source, followed by dispersion. Third stage shows the most pronounced form of plume. Significant concentrations are transported a considerable distance from source in direction of wind propagation, followed by dispersion.

Opposed to case when mouth of source is located below the lower boundary of inversion layer, which is shown in Figure 10, significant concentrations are transferred on shorter distance from source.

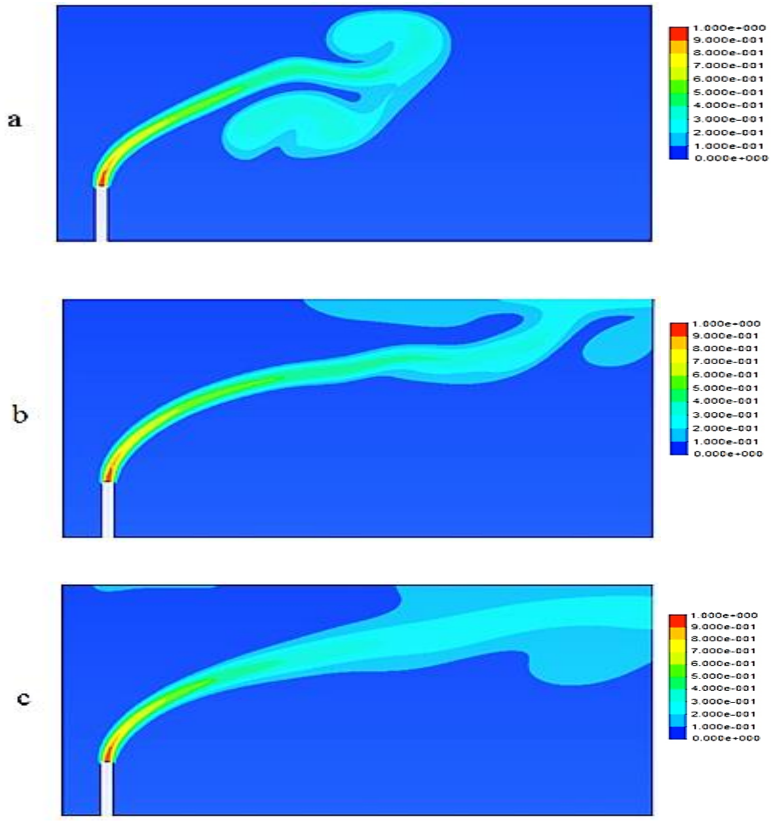


Figure 9. Temporal distribution of methane (CH_4) concentration in case when the lower boundary of inversion is located above mouth of source

It can be seen how plume acquires more pronounced cone shape over time. In comparison with Figure 10, it can be noted that dispersion of harmful substances is greater, which is due to fact that plume enters the atmosphere layer, where temperature gradient is positive. It can also be noted that in case when inversion layer is below mouth of source, significant concentrations of harmful substances are observed at higher altitude than when inversion layer is located above mouth of source.

Figure 10 shows methane concentration distribution emitted by point source at velocity of 10 m/s over time (t = 10 s (10 (a)), t = 30 s (10 (b)), t = 60 s (10 (s))), taking into account that mouth of source is located below the lower boundary of inversion layer. In contrast to the case when mouth of source is located above the upper boundary of inversion layer, which is shown in Figure 9, significant concentrations are transferred to a larger distance from source. It can also be noted that dispersion of harmful substances is less, which is due to fact that plume enters to inversion layer, which prevents diffusion. In case when inversion layer is below mouth of source, significant concentrations of harmful substances are observed at lower altitude than when inversion layer is located above mouth of source.

According to this, it can be argued that the case where inversion layer is located below mouth of source is safer for ecology of ground layer.

Conclusion

Thus, the computational model is constructed to determine expansion of harmful impurities in ground layer in different temperature stratification based on ANSYS software. Numerical experiments are conducted for different pollutant-emission rate from point source, for different temperature stratifications with altitude, which makes it possible to predict flame contour and its extent.

Obtained results can be used to predict distribution of concentration in ground layer, quality of air composition, that has a significant effect on state of environment ecology. Analyzing the obtained results makes possible to note the necessity of creating similar models for predicting the distribution of harmful substances concentration in ground layer, which will affect the state of environment ecology in general, and of atmosphere in particular.

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