4-бөлім	**Раздел 4**	**Section 4**
Қолданбалы математика	**Прикладная математика**	**Applied Mathematics**

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NUMERICAL SIMULATION OF CONTAMINANTS TRANSPORT IN HUMAN SETTLEMENTS TAKING INTO ACCOUNT CHEMICAL REACTIONS

In this paper, we performed a numerical simulation of the spread of pollutants due to a chemical reaction near the roadway inside an urban street canyon. In the course of our study, we studied the dispersion properties of the gas when it collides with the idealized buildings that make up the urban canyon. In conclusion, a qualitative assessment was given that characterizes the nature of the distribution of the concentration of the pollutant and the process of the appearance of zones with increased turbulence, in which vortices are formed that interfere with the ventilation properties of the horizontal flow, which significantly affects the health and life of people. NO and NO_2 released into the canyon area were chosen as the considered reactive substances, and ozone O_2, which is present in the moving air stream, was chosen as the third reactive substance. The results obtained can be used in the future for use by transport designers and road engineers, whose goal is to reduce the concentration of nitrogen oxides near the pedestrian zone of the city. All the results obtained were first tested on test problems, the results of which are in excellent agreement with the numerical and experimental values of other authors.

Key words: urban street canyon, turbulent model, Navier-Stokes equations, LES model, chemical reaction, air pollution, concentration, polluting emission, ozone.

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Химиялық реакцияларды ескере отырып, елді мекендерде ластаушы заттардың тасымалдануын сандық модельдеу

Бұл жұмыста қалалық көше каньонының ішіндегі жолдың жанында химиялық реакция нәтижесінде ластаушы заттардың таралуын сандық модельдеу жүргізілді. Біздің зерттеу барысында қалалық каньонды құрайтын идеализацияланған ғимараттармен соқтығысқан кезде газдың дисперсиялық қасиеттері зерттелді. Осы жұмысты қорытындылай келе, ластаушы концентрацияның таралу қозғалысы мен бағытын сипаттайтын нәтижелері берілді және көлденең ағынның желдету қасиеттеріне кедергі келтіретін құйындар пайда болатын турбуленттілігі жоғары аймақтардың пайда болу процесі талданды және де бұл адамдардың денсаулығымен өміріне айтарлықтай әсер ететінін дәлелдеді. Қарастырылған химиялық белсенді заттар ретінде каньон аймағына шығарылатын NO және NO_2 таңдалды, және де үшінші реактивті зат ретінде қозғалатын ауа ағынының құрамында болатын озон O_2 таңдалынып алынды. Қала жаяу жүргіншілер аймағына жақын таралатын улы газдардың, яғни азоттоксидінің концентрациясын төмендету мақсаты болып табылатын көлік жобалаушыларымен жол инженерлерінің пайдалануы үшін алынған нәтижелерді пайдалануға болады. Алынған барлық нәтижелер алдымен тест тапсырмаларында сыналып зерттелді және де олардың нәтижелері басқа да ғалымдардың жұмыстарымен салыстырылып, олардың сандық және эксперименттік нәтижелері жақсы сәйкестік көрсетті.

Түйін сөздер: қалалық көше шатқалы, турбулентті модель, Навье-Стокс теңдеулері, LES моделі, химиялық реакция, ауаның ластануы.

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Численное моделирование переноса загрязняющих веществ в населенных пунктах с учетом химических реакций

В настоящей работе было произведено численное моделирование распространения загрязняющих веществ вследствие протекания химической реакции вблизи проезжей части внутри городского уличного каньона. В ходе нашего проведенного исследования были изучены дисперсионные свойства газа при столкновении с идеализированными зданиями, составляющими городской каньон. В заключении была дана качественная оценка, характеризующая характер распространение концентрации загрязнителя и проанализирован процесс появления зон с повышенной турбулентностью, в которых образовываются вихри, препятствующие вентиляционным свойствам горизонтального потока, что в значительной степени сказывается на здоровье и жизнедеятельности людей. В качестве рассматриваемых химически активных веществ были выбраны NO и NO_2, выбрасываемые в область каньона, третьим реакционным веществом был выбран озон O_2, присутствующий в составе движущегося потока воздуха. Полученные результаты могут быть использованы в дальнейшем для использования транспортными проектировщиками и дорожными инженерами, целью которых является снижение концентрации оксидов азота вблизи пешеходной зоны города. Все полученные результаты были сначала апробированы на тестовых задач, результаты которых отлично согласуются с численными и экспериментальными значениями других авторов.
Ключевые слова: городской уличный каньон, турбулентная модель, уравнения Навье-Стокса, модель LES, химическая реакция, загрязнение воздуха.

1 Introduction

Every year, with the growth of technological progress and widespread urbanization of cities, we can observe a colossal increase in vehicles and the growth of industrial zones, which in turn led to the maximization of daytime traffic and a commensurate increase in the concentration of exhaust gases in the pedestrian zone [1], [2]. Transport is a source of toxic gases such as sulfur dioxide SO_2, nitrogen N_2, nitrogen oxides NO_x, carbon monoxide CO, carbon dioxide CO_2, aldehydes, heavy metal compounds, benzene C_6H_6, carcinogenic benzopyrene C_2OH_12, as well as particulate matter and soot hazardous to health. The height of the building in the street canyon is much greater than the width of the road, which creates a harmful environment in the space without air circulation due to weak gusts of wind. The high concentration of pollutants from exhaust gases in the air pool is harmful to human health, especially asthma, chronic diseases of the digestive, cardiac, nervous and respiratory systems [3]. Tominaga Y., Stathopoulos T. [4], [5] conducted a number of studies to study the mechanism of the formation of pollutants in the pedestrian zone. In these studies, wind tunnel experiments were performed and numerical simulations were performed using computational fluid dynamics (CFD).

One of the most ambitious problems in the field of chemical reactions is the interaction of ozone with NOx molecules: as you know, the air contains a fraction of ozone, which periodically interacts with nitrogen mono- and dioxides, entering into an exchange reaction. The resulting substances have a detrimental effect on the health of all living organisms. This problem has been studied by Carpenter, L.J., Clemitshaw, K.C. [6], in addition, recommendations and analysis of the quality of the air in the areas adjacent to the canyon were given. Also in Baker, J., et al. [7] took into account the photochemical properties of the ongoing reactions. In studies Zhong J. et al. [8] the numerical results that were solved using the LES model coincide with the experimental values. Also, with the LES model, good results were seen for the emerging product with a compound of ozone O3 and nitrogen oxide NO. This problem was studied by Kim M. et al. [9]. The paper [10] examines the sensitivity of O3 to NOx and VOC emissions. This study is an attempt to analyze the spread of dozens of reactive pollutants in and over a street canyon using a CFD model.

In this article, numerical results were presented, in which the course of a chemical reaction was considered, a comparative analysis of the results obtained with experimental data was made, after which a qualitative conclusion was made about the consistency of the obtained data with empirical values. In the task, a mixture of ozone with carbon monoxide was investigated, which, as a result of chemical reactions, decomposes into carbon dioxide and oxygen. All numerical calculations were carried out in an idealized street canyon, which consists of two buildings, in addition, a pollutant emerges in the middle of the street along the entire length of the roadway.

2 Formulation of the problem

Denev J, A., Frohlich J., Bockhorn H. [11] carried out a direct numerical simulation (DNS) of a transverse flow with a jet emerging from a circular cylindrical tube; as a result of collision of flows, a chemical reaction occurs in the forward direction. This simulation was calculated with a small value of the Reynolds number, equal to $Re = 275$. For the study, a three-dimensional model of a microreactor was built in the center, consisting of two transverse flows. All dimensions are reduced to dimensionless, with the value of the pipe diameter, where $D = 8mm$ (D is the pipe diameter). The vertical axis is located at a $3D$ distance from the horizontal axis. Height and width of horizontal pipe $13,5D$, length $20D$, pipe height $2D$. The tube configuration is shown in detail in figure(Рис.1).

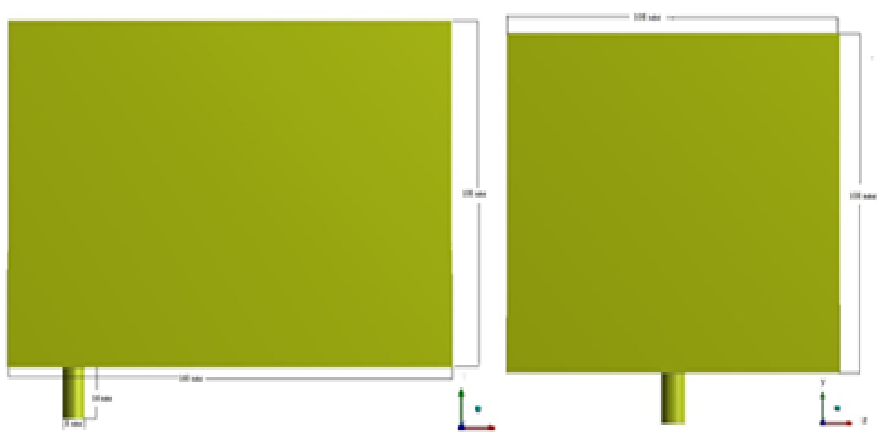

Figure 1: Parameter of the calculated area

An unstructured mesh was created for the simulation. In the geometry, a computational subdomain was created, to which the mesh was refined, the location of the subdomain was chosen near the cylindrical pipe. The total number of elements is 1104850, the number of nodes is 192787. Figure (Рис.2) show the groups of the studied territories.

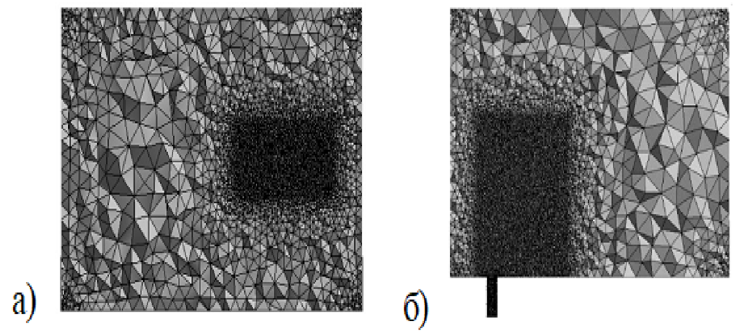

Figure 2: Through the calculated area in the plane (a) XOZ (b) XOY

Damkehler's number $Da = 1.0$ is chosen so that the simulation estimate is available. As the calculated indicators in the calculation, it was assumed that the kinematic viscosity of air $\nu = 1.40610^{-5}$ m^2/s, density $\rho = 1.225$ kg/m^3, velocity is $u = 0.48$ m/s. All values are obtained empirically and are completely physical [12].

3 Materials and Methods

Determination of the reactive flow velocity with the main velocity is denoted as $R = U_{b,jet}/U = 2.42$. The volumetric flow rate is $U_{b,jet} = 1.16$ m/s. The flow velocity from the cylindrical pipe is characterized by the following velocity profile:

$$w\left(r\right)/U_{b,jet} = 2\left[1 - \left(r/\left(D/2\right)^2\right)\right], \tag{1}$$

here, r - is the radial coordinate, w - is the vertical velocity component. The velocity profile at the flow boundary can be described as follows:

$$u\left(d_n\right) = 1.0 - \exp(-3.0 d_n), \tag{2}$$

here, d_n - the closest distance to the channel wall, that is [11]:

$$d_n = min(x, L_x - x). \tag{3}$$

All limited conditions The reference area is shown in more detail in the pictures(Рис.3).

In this work, the numerical results were compared with the experimental and numerical values of Denev J, A. [11]. Figure (Рис.4) shows the average velocity of the horizontal velocity component.

Figure (Рис.5) shown is the average speed v of the speed component. The figure (Рис.5) compares the profiles of the middle conceptions of the B version, with a freely selectable

To solve the problem inside the urban canyon, the study by Baker, J. [7] was used. It was accepted that $H/W = 1$. When creating a computational model, a three-dimensional

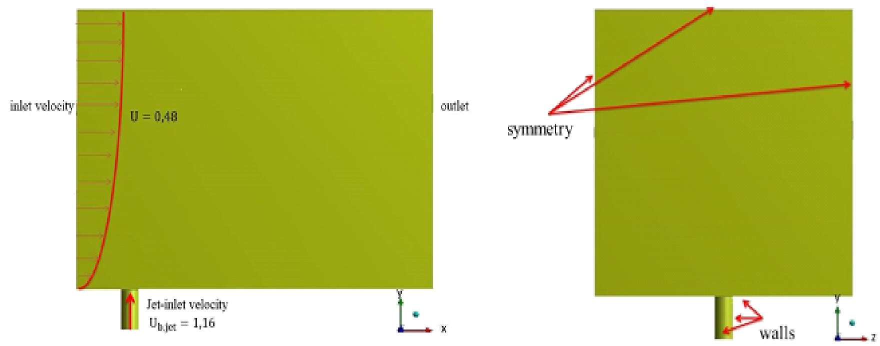

Figure 3: Basic conditions for the vertical view of the reactor in the OXY plane; Basic conditions of the vertical view of the reactor in the plane of OYZ

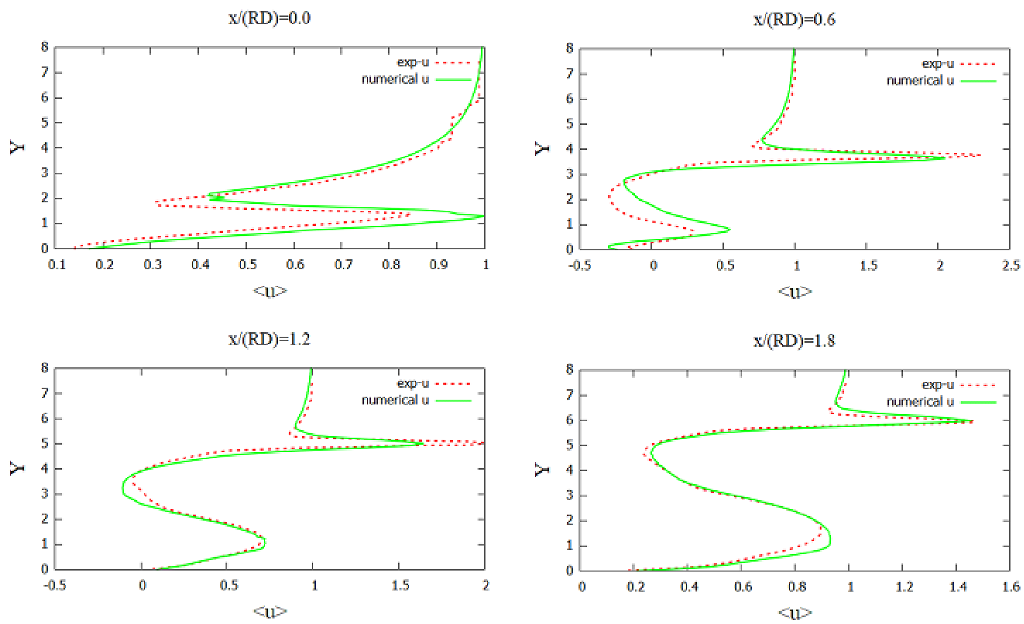

Figure 4: Comparison of the profiles of the average velocity u at the indicated points

computational domain was adopted. Figure (Рис.7) 8 illustrates the configuration of the computational domain. The height of the buildings is the same and equal to the value of $H = 18$, the width of the canyon is equal to $W = 18$. In the center of the pedestrian part, there is a source of pollutant, 0.3 m by 0.3 m in size. Gas CO and NO, come out of the source, which enters into a chemical reaction with ozone O_3, moving in a cross-flow.

$$O_3 + NO = NO_2 + O_2 \tag{4}$$

$$O_3 + CO = CO_2 + O_2 \tag{5}$$

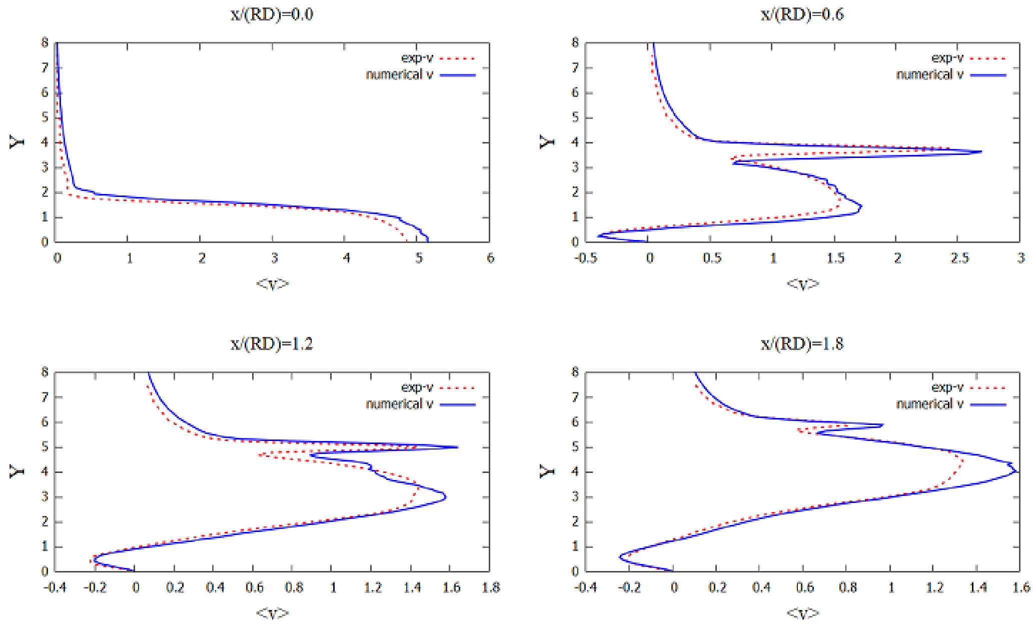

Figure 5: Comparison of the profiles of the middle v speed components at the specified points

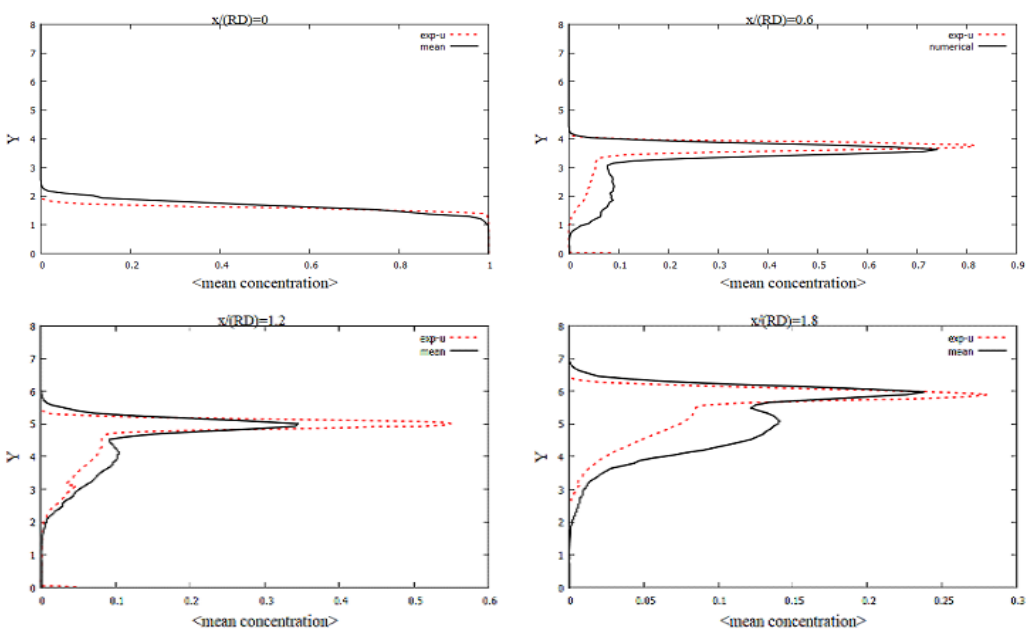

Figure 6: Comparison of the profiles of the mid-range values ??of the time B

Unlike the initial gases, the reaction products have a detrimental effect on the health of living organisms, as a result of which the substitution reaction is the object of close study.

Figure (Рис.8) shows an image of the computational domain. Thickening was carried out along the street of the canyon at a height of 30 above the source of pollution. The total

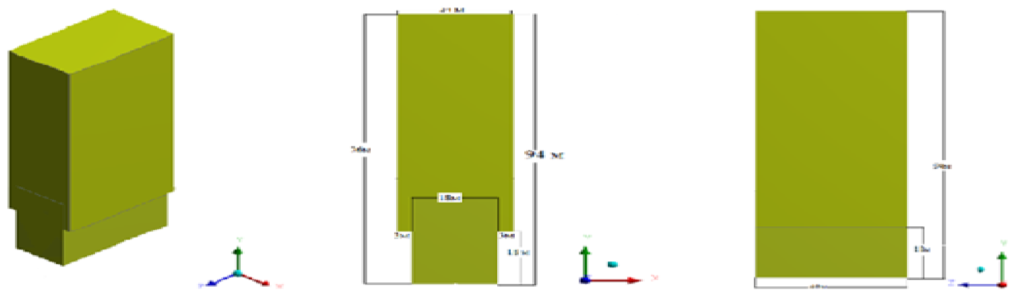

Figure 7: 3D model of the investigated term; Parameter of the calculated range from the XOY and YOZ planes

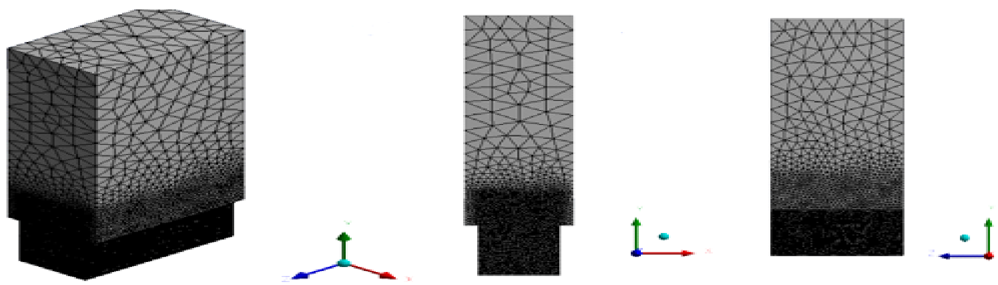

Figure 8: Powerful area

number of elements and nodes is 1526580 and 264265 respectively.

4 Numerical results

The study was carried out using the ANSYS Fluent. The time step size is 1. The total computation time was one hour, and the result was visualized. The LES model was used in conjunction with calculations of the chemical reaction caused by pollutants within the canyon. The numerical calculation was carried out using the SIMPLE algorithm (partially closed method for pressure-dependent equations).

The chemical reaction was solved using the Smagorinsky model. Smagorinsky's constant is equal to $C_s = 0.1$. According to reaction (4) figure (Рис.9) shows the mass fraction of mean concentrations in the windward and lateral relief of NO, NO_2, O_3.

The mass fraction profile of the average concentration of CO, CO_2 and O_3 -coating at a height of 0,3 m from the pollution source is shown in figure (Рис.11). According to reaction (5) figure (Рис.11) shows the mass fraction of the average concentrations of CO, CO_2 and O_3 in the windward and lateral relief. In figures (Рис.10) and (Рис.12) the detection of pollutant concentrations was visualized using ANSYS Fluent Volume Rendering.

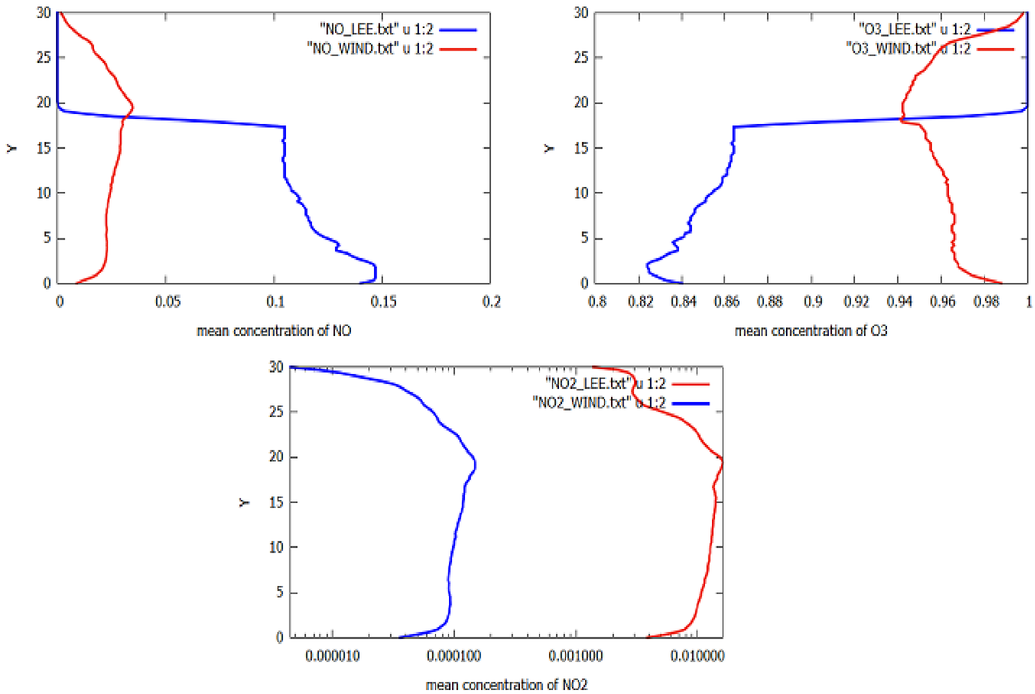

Figure 9: Equivalence of the mass content of the average concentrations of the nitric oxide, the ozone and the dioxide of the nitrogen oxide in the current $z/H = 0$

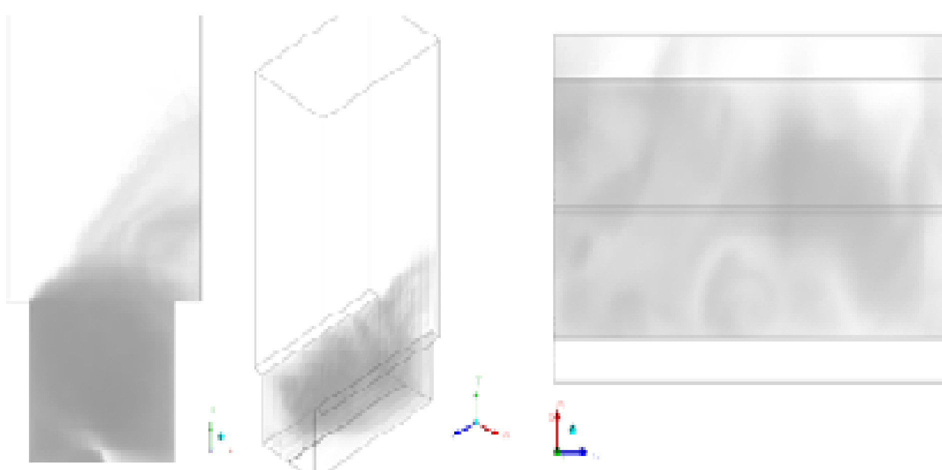

Figure 10: Distribution of concentration NO_2

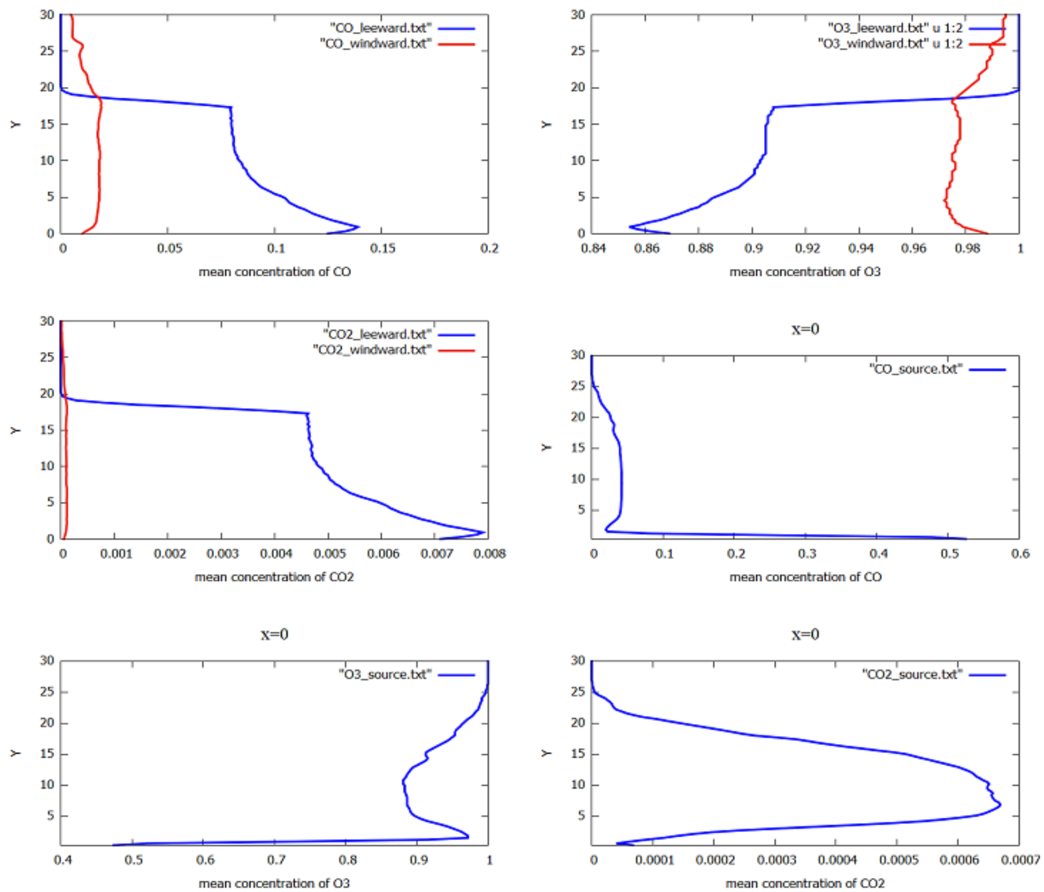

Figure 11: Comparison of the concentration of the upwind and leeward headlands at the point $z/H = 0$ and the concentration of the pollutant , $_3$, $_2$ at the point $z/H = 0$

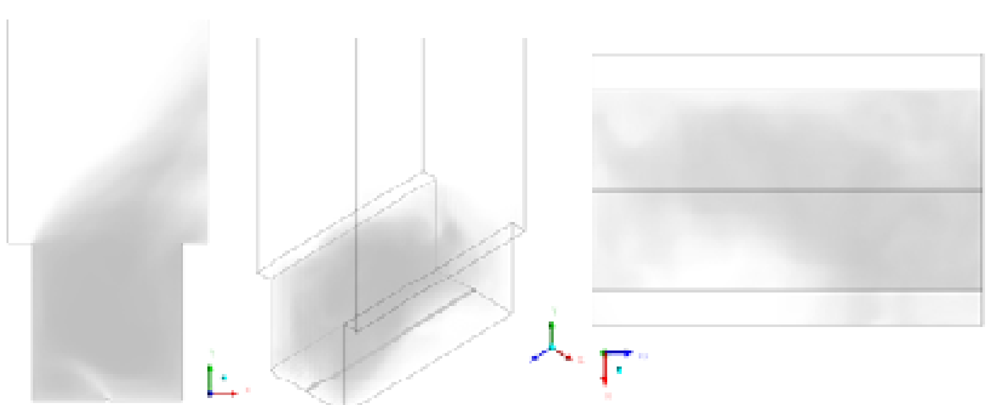

Figure 12: Distribution of concentration CO_2

5 Conclusion

At the beginning of the work, a literature review was carried out on modeling the chemical reaction that occurs when pollutants from vehicles are detected in the city street gorge in order to identify the main problems in this industry. A mathematical model was developed to describe the flow. To ensure the correctness of the mathematical model and numerical algorithm, the test problem was solved using the ANSYS Fluent software package. The results of the study show that to check the growth rate and determine the mass of the formed chemical products of a chemical reaction, a test task was performed, and then checked and compared with the results of experimental and numerical studies by well-known authors; the search for the most efficient turbulence model was carried out; the geometry of the real dimensions of the city street canyon was created, divided into groups and the computational domain was condensed; reactive substances NO, CO, interacting with ozone from the source of pollution and emitting toxic gases such as NO_2, CO_2, harmful to human health, were quantified and visualized.

In street canyons, depending on the length of buildings and the configuration of the street, gases such as NO_2, CO_2, are dispersed, which leads to disruption of the normal circulation of the wind flow. Even in the gorge, this leads to an increase in temperature and an accumulation of concentrations of life-threatening gases. The direction of the wind can change and intensify, causing a hurricane. In addition, the slope of the gorge is 4 times more polluted with ultrafine particles than the wind slope. This means that the most polluted air is breathed in the pedestrian zone. The research results can be applied to numerical modeling in the future to solve new questions and problems in the studied area of knowledge.

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