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NUMERICAL MODELING OF CONTAMINATING SUBSTANCES DISTRIBUTION IN RESIDENTIAL AREAS

Abstract. In this study, a numerical simulation of the contaminants distribution in a street canyon and the effect of barriers on this process were carried out. To solve this problem, a Reynolds-averaged Navier-Stokes equation was used. To solve this problem, a turbulent DES model was used, which showed good results for the test problem. To test the mathematical model and the numerical algorithm, the test problem was solved. The obtained numerical results were compared with experimental data and the results of modeling by other authors. After checking the mathematical model and the numerical algorithm, the main problem was described considering the process of pollutant emission between houses using different barrier heights. As a computational area, a model of a street canyon was taken with a ratio of sides that ranged from 0.05 m to 0.2 m. As shown by numerical modeling, the presence of barriers leads to the appearance of an additional vortex in the space between objects, which increase as their height increases. As a result, it can be observed that most of the contaminants are trapped between them. In the course of various studies it was revealed that the presence of barriers along the roads reduces the concentration of harmful substances in the air. So when using a grass barrier height of 0.1 m, the concentration value falls into the section x=0.05 m more than 1.5 times as compared without using barriers. Thus, it can be said that barriers provide good filtration of polluted air, which has a detrimental effect on the environment and human health.

Keywords:air pollution; pollutantsdispersion; concentration fluctuations; high concentration; transport; urban street canyon.

1. INTRODUCTION

Today, statistically, it can be observed the high level of an urbanization that led to the fact that people began to move more often to the large cities with rich infrastructure. All this caused rapid growth of urban population around the world which only amplified with development of science and technology. If in the middle of the last century the rural population were twice more than urban, then in 1990 43% of world's population lived in the cities, and these are 2.3 billion people. By 2015 this number grew to 54% or 4 billion people, and, according to forecasts, by 2030 about 60% of world's population will live in the cities [1]. Big cities involve the high level of pollution to the environment as in the large cities, the main source of air pollution (70-80%) are exhaust gases of cars, with growth of urban population the number of harmful emissions in the atmosphere sharply increases. High air pollution considerably increases incidence of the population. In this regard, the purpose of this work is studying of pollutants distribution in the cities and influence of acoustic barriers on this process.

A large number of researches were conducted to study this problem. For example, in research influence of stability conditions of the atmosphere on pollutants distribution of city canyons [2] which showed that at emergence of an air pollution source it was observed instability of air flow, the involving emergence of a whirlwind between buildings on site of collision of two flows. In other paper [3] was estimated influence of different conditions to temperature stratification on pollutants distribution near the uninsulated multi-storey building. From all numerical models, according to results, the LES model gives more exact forecasts of speed for neutral conditions, than for others. Also influence of billboards on pollutants distribution on streets with a different party'sratio of H/W where W – width of a canyon, H –

height of a canyon was estimated [4]. The case with H/W=2 shows smaller concentration of pollutants, than a case with H/W=1. With a versatile source vertical and two-layer billboards result in larger concentration, than side and single-layer.

In paper [5] was applied k-ε turbulent model to an influence research at presence of the buildings located against wind on pollutants distribution in the multi-storey building. According to results, existence of buildings above on a current has a significant positive effect on ventilation of the building at the oblique winddirection, than at normal impact of wind as they have an insignificant impact. In other similar research [6] authors applied the LES model to studying of the air pollution impact caused by cars on air quality in rooms of buildings with natural ventilation in close proximity to the carriageway. In this work influence of such factors as distance from the carriageway to the building, the wind speed, particle size, arrangement and the size of a window were studied.

In paper [7] dispersion of the pollutants which are thrown out from a source on the bottom of a city canyon caused only by thermal buoyancy force created by the heated outside surfaces of the building and a bottom of a street canyon was investigated. They also considered how the different horizons (skylines) will influence deduction of pollutants in city canyons. In paper [8] was carried out computational modeling of pollutants dispersion in canyons with different ratios of the parties with using DES. This research shows that for street canyons with W/H=1 and W/H=2 the upper corner of a leeward wall will be a zone of the contaminating impurityaccumulation, and in case of W/H=2 such zone can arise in the middle of the lower part of a canyon. In paper [9] was applied LES to define whether it is possible to classify flow models on some identified modes in a three-dimensional canopy of the city building and to define the main features of distribution of pollutants in the different modes of a flow.

Also influence of chemical reactions, chemically active pollutants on structure of a flow and dispersion of pollutants was investigated. In paper [10] was conducted a research to study influence of bimolecular reactions and city configurations on concentration and transfer of pollutants of air at the city microlevel. The LES model in combination with second ordered speed constant model was used for computer simulation. In the paper [11] developed and implemented a computational model of hydrodynamics in combination with the mechanism of carbon communications of IV (CBM-IV) for studying of chemically active pollutants dispersion in urbanareas. With use of this model dispersion of reactive pollutants in a street canyon above with a ratio of the parties of equal 1 m is investigated.

In paper [12] the research for definition influence of computing parameters, such as permission of a grid, step size on time, on characteristics of Navier-Stokes's (RANS) equations with Reynolds-averaged stability model, a method of large vortex method (LES) and model with the deferred vortex simulation (DES) was conducted. According to results, the LES model gives the most exact forecast of pollutants distribution in comparison with results of an experiment in the wind tunnel. In the paper [13] used the system of modeling Quick Urbanand Industrial Complex (QUIC) for a research of influence of buildings presence on dispersion of exhaust gases in the city. In point comparison concentration of vehicles emission was usually higher for a case with buildings because ofthe increased holding time of pollutants in street canyons. However, it is possible to observe the return when concentration in all area was on average lower for a case with buildings.

Influence of trees presence on distribution of pollutants was investigated in paper [14]. Authors developed new structure (framework) of modeling, the connecting LES and Lagrangian stochastic model (LSM) for this purpose. Results of this research showed that trees which are higher than building height, have the most considerable impact on distribution of pollutants and on air flow in general.

There were many experiments on a research of flow structure in city street canyons. In paper [15] made an experiment to investigate interaction between inertially managed flow caused by surrounding winds, and the flow caused by force of buoyancy and uneven walls heating of a canyon.

2. Mathematical model

Computer simulation was carried out with use of the DES model which represents a combination of the LES and RANS models. The LES method is used for modeling of certain areas of a flow, and RANS for an interface. The new parameter determinedas $d = \min(d, C_{des}\Delta)$ where $\Delta = \max(\Delta x, \Delta y, \Delta z)$ is the large scale of a cell of a grid, and C_{des} - empirical values, in our case equal 0.61, guarantees the correct switching of the modes between LES and RANS.

Main equations of the LES model:

$$\frac{\partial \overline{u_l}}{\partial x_i} = 0$$

$$\frac{\partial(\rho\overline{u_l})}{\partial t} + \frac{\partial(\rho\overline{u_i u_J})}{\partial x_j} = -\frac{\partial \overline{p}}{\partial x_j} + \vartheta\frac{\partial^2 \overline{u_l}}{\partial x_i^2} - \frac{\partial \tau_{ij}}{\partial x_j}$$

$$\frac{\partial(\rho\overline{c})}{\partial t} + \frac{\partial(\rho\overline{u_J c})}{\partial x_j} = -\frac{\partial J_j}{\partial x_j}$$

where u_i and u_j components of speed, ρ – pressure, ρ – density, with – concentration of the contaminating impurity and ϑ – viscosity. RANS was used in an interface for increase in accuracy of modeling near a wall. It was used the Realizable $k-\varepsilon$ model which is improvement of the Standard $k-\varepsilon$ model. Kinetic energy of turbulence is defined as:

$$\frac{\partial}{\partial t}(\rho k) + \frac{\partial}{\partial x_j}(\rho k u_j) = \frac{\partial}{\partial x_j}\left[\left(\mu + \frac{\mu_t}{\sigma_k}\right)\frac{\partial k}{\partial x_j}\right] + \mathrm{P}_k + \mathrm{P}_b - \rho\varepsilon - Y_M + S_k$$

$$\frac{\partial}{\partial t}(\rho\varepsilon) + \frac{\partial}{\partial x_j}(\rho\varepsilon u_j) = \frac{\partial}{\partial x_j}\left[\left(\mu + \frac{\mu_t}{\sigma_\varepsilon}\right)\frac{\partial \varepsilon}{\partial x_j}\right] + \rho C_1 S_\varepsilon - \rho C_2 \frac{\varepsilon^2}{k + \sqrt{\nu\varepsilon}} + C_{1\varepsilon}\frac{\varepsilon}{k}C_{3\varepsilon}P_b + S_\varepsilon$$

where

$$C_1 = \max\left[0.43, \frac{\eta}{\eta+5}\right], \eta = S\frac{k}{\varepsilon}, S = \sqrt{2S_{ij}S_{ij}}$$

Turbulent viscosity:

$$\mu_t = \rho C_\mu \frac{k^2}{\varepsilon}$$

where

$$C_\mu = \frac{1}{\mathrm{A}_0 + \mathrm{A}_S U * \frac{k}{\varepsilon}}$$

$$U^* = \sqrt{S_{ij}S_{ij} + \widetilde{\Omega}_{ij}\widetilde{\Omega}_{ij}, \widetilde{\Omega}_{ij} = \Omega_{ij} - 2\varepsilon_{ijk}\omega_k, \Omega_{ij} = \overline{\Omega_{IJ}} - \varepsilon_{ijk}\omega_k}$$

Where (Ω_{ij}) the tensor of average speed of rotation observed in the frame of reference rotating with angular speed ω_k. A_0 and A_s is defined as:

$$\mathrm{A}_0 = 4.04, \mathrm{A}_S = \sqrt{6\cos\phi}$$

$$\phi = \frac{1}{3}\cos^{-1}\left(\sqrt{6W}\right), W = \frac{S_{ij}S_{jk}S_{ki}}{\widetilde{S}^3}, \widetilde{S} = \sqrt{S_{ij}S_{ij}}, S_{ij} = \frac{1}{2}\left(\frac{\partial u_j}{\partial x_i} + \frac{\partial u_i}{\partial x_j}\right)$$

Model constants:

$$C_{1\varepsilon} = 1.44, C_2 = 1.9, \sigma_k = 1.0, \sigma_\varepsilon = 1.2$$

3. METHOD OF SOLUTION

It was used a semi-implicit method for the equations connected with pressure, or SIMPLE [16-19] for correction of pressure. The SIMPLE method was developed and presented by Spalding and Patankar [16].

4. DESCRIPTION OF AN EXPERIMENT

It is supposed that the direction of wind is perpendicular to a street canyon. Circulation in a canyon is caused by a flow over a canyon. In the lower part of the camera center the line of a source of pollutants as in figure 1 was placed.

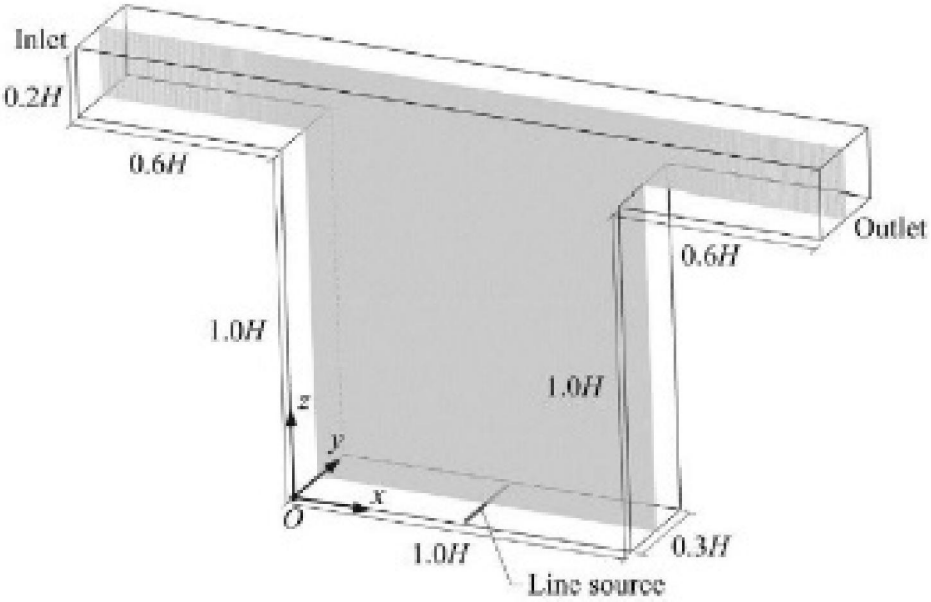

Figure 1– Geometry of a test problem

A mixture of air and ethylene C_2H_4 with a concentration of 1.2% was used as pollutants. The speed of the air flow over the canyon was equal to 1 m/s, the speed from the linear source was equal to 0.1923 m/s.

5. COMPUTATIONAL MODELING

As estimated area the model of a street canyon with the ratio of the parties equal to 1 was used. As in this research it wants to estimate influence of barriers presence on distribution of pollutants, it was needed to add a wall for their modeling. Such walls are located as on the right, and to the left of the line of a source. Modeling was carried out for 3 different heights of barriers: 0.05 m, 0.1 m and 0.2 m.

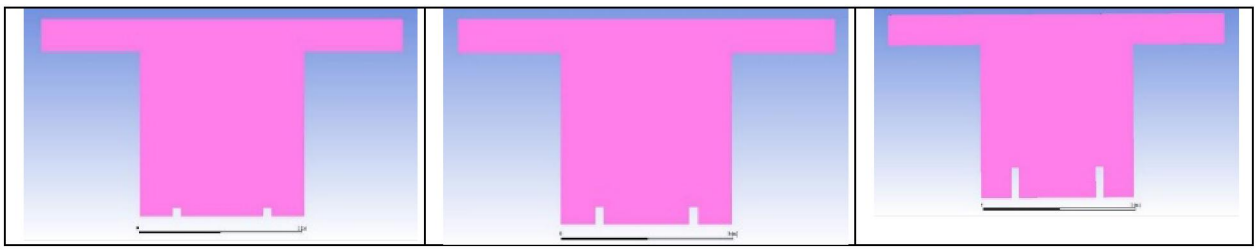

Figure 2 – Task geometry with different type of a barrier with height

Computer simulation was carried out on Ansys 18.0 on a heterogeneous grid with a scale which will increase from a bottom up to top of geometryfield. The space near the line of a source has the smallest slot

pitch equal to 1 m, and the space over a canyon has slot pitch of 5 m. Thus, grids for these three geometries have 3706717, 3921432 and 4357700 elements for height of a barrier of 0.05 m, 0.1 m and 0.2 m respectively, as in figure 2.

6. RESULTS AND DISCUSSION

In figure 3 mean values of velocity components on for all the time of calculation is represented.

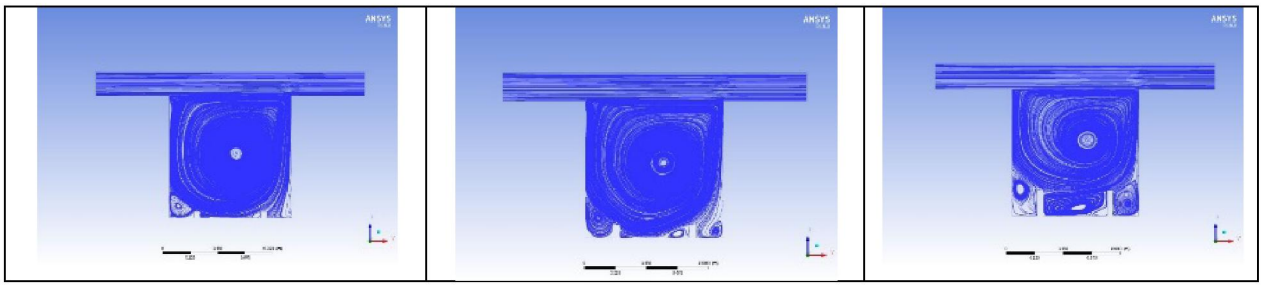

Figure 3 – Mean value of components of speed

In figure 4 lines of current for different heights of barriers are represented. It is possible to notice how in process of increase in height of barriers new whirlwinds appear and amplify. Thus for h=0.2 m flow direction near a source of the contaminating impurity changes on opposite.

In figure 5 distribution of concentration of the contaminating impurity in a street canyon where it is visible that with a barriers height of 0.2 meters concentration of pollutant between barriers considerably increases in space is represented.

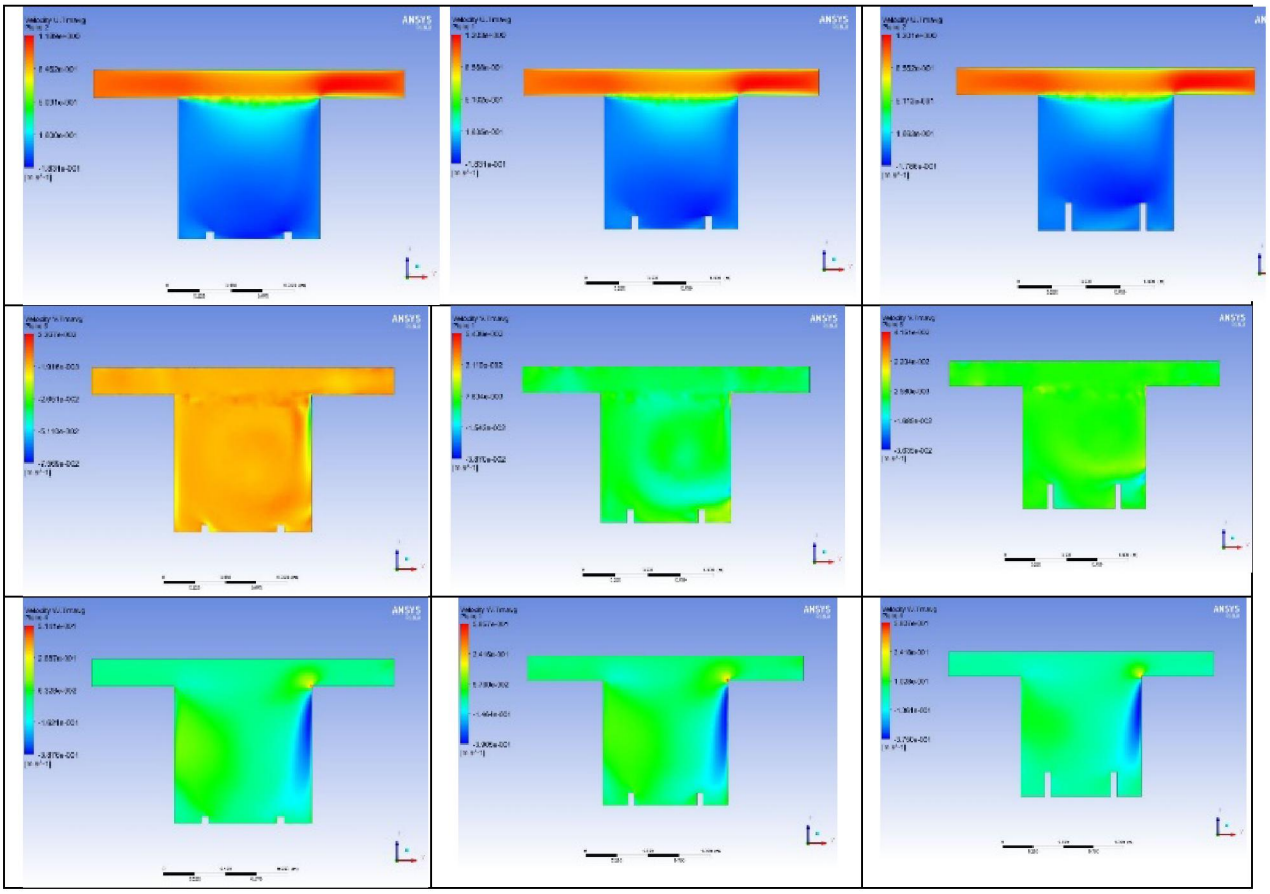

Figure 4 – Lines of current for different heights of barriers

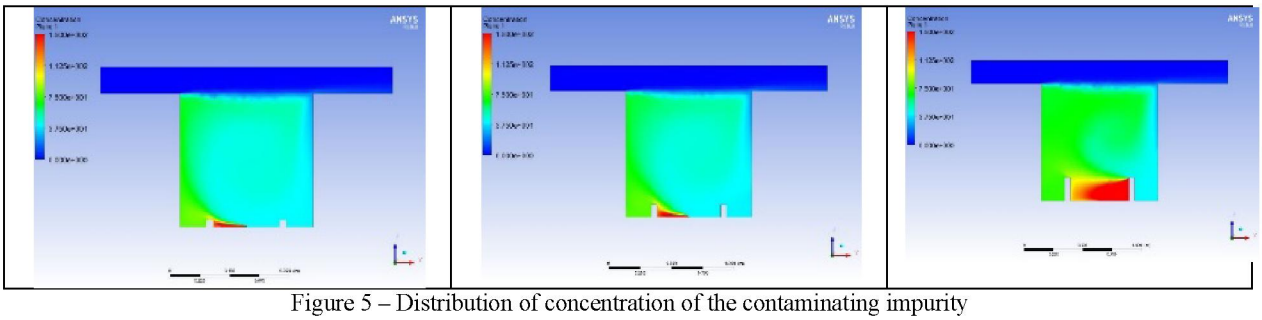

Figure 5 – Distribution of concentration of the contaminating impurity

In figure 6 it is shown a velocity profile. In figure 7 the concentration profile is represented. Apparently, from drawings barriers reduce concentration of the contaminating impurity approximately twice at X=0.05 m, and leads to insignificant increase in concentration at X=0.95 m. At the same time whenbarrier height of 0.2 m the most part of pollutant remains in space between barriers and in general reduces concentration near houses.

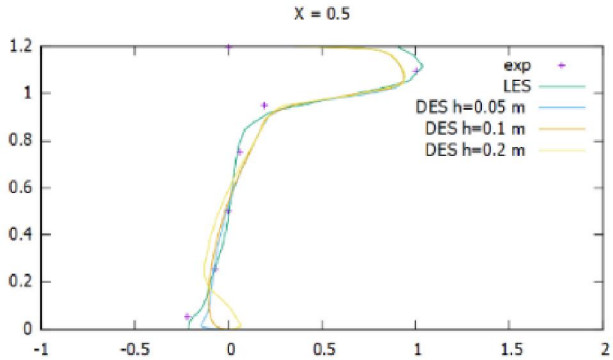

Figure 6 – Speed profile

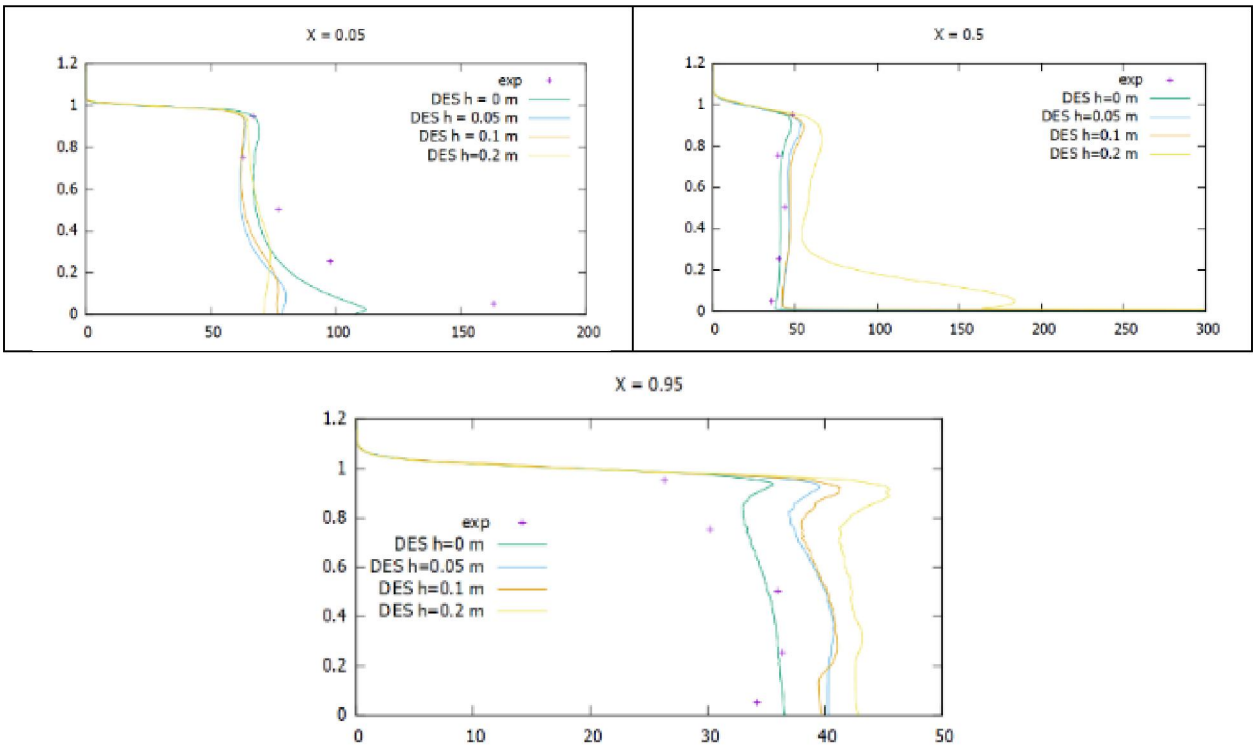

Figure 7 – Concentration profile for different sections

7. CONCLUSION

Computational modeling of the contaminating impurity distribution in a street canyon with barriers to different heights was carried out. For computational modeling the DetachedEddySimulations (DES) model which showed good accuracy at a solution of a test problem was selected. To check model the test problem, results which showed that the selected model is suitable for computational modeling was solved.

As show results of modeling, existence of barriers has significant effect on distribution of the contaminating impurity. Concentration of impurity on leeward of a canyon decreases approximately twice, and from less windy party slightly increases though apparently from the received diagrams it is still twice lower, than on leeward. At the same time concentration of pollutant between barriers considerably increases in space. Proceeding from it is possible to tell that barriers provide protection of houses not only against noise, but also against the contaminating impurity which are thrown out air vehicles.

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ТҰРҒЫН ҮЙ АУМАҒЫНДАҒЫ ЛАСТАУШЫ ЗАТТАРДЫҢ ТАРАЛУЫНЫҢ САНДЫҚ МОДЕЛДЕУІ

Аннотация. Бұл зерттеуде көше каньонындағы ластаушы заттардың таралуын сандық моделдеу және осы үдеріске кедергілердің әсері жүргізілді. Бұл мәселені шешу үшін Рейнольдс орташаланғаны бойынша Навье-Стокс теңдеуі қолданылды. Бұл мәселені шешу үшін DES турбуленттік моделі қолданылды,ол тест тапсырмасы үшін жақсы нәтижелер көрсетті. Математикалық модельді және сандық алгоритмді тексеру үшін тест тапсырмасы шешілді. Алынған сандық нәтижелер эксперименталдық деректермен және басқа авторлардың үлгілеу нәтижелерімен салыстырылды. Математикалық модельді және сандық алгоритмді тексергеннен кейін үйлер арасындағы ластаушы заттардың эмиссия процесін есепке ала отырып, кедергілердің әр түрлі биіктіктерін пайдалануда негізгі міндеттері сипатталған.0,05 м-ден 0,2 м-ге дейінгі диапазондағы аралығында арақатынасы бар көше каньонының моделі есептік аймақ ретінде алынды. Сандық үлгілеу көрсеткендей, кедергінің биіктігінің өзгеруіне байланысты, кедергілердің болуы объектілер арасындағы кеңістікте қосымша құйынды пайда болуына алып келеді. Нәтижесінде ластаушы заттардың көпшілігі олардың арасындағы тұзаққа түсетінін байқауға болады. Әр түрлі зерттеулер барысында жол бойындағы кедергілердің болуы ауадағы зиянды заттардың концентрациясын төмендететіні анықталды. Сондықтан биіктігі 0,1 м шөп кедергісін пайдаланған кезде шоғырлану мәні x=0,05 м қимасында тура келеді, кедергілерді пайдаланбай-ақ салыстырғанда 1,5 еседен азаяды. Осылайша, қоршаған орта мен адам денсаулығына зиянды заттардың әсер етуін алдын алуға және кедергілер ластанған ауаны жақсы сүзуді қамтамасыз ететінін айтуға болады.

Түйін сөздер: ауаның ластануы; ластаушы заттардың дисперсиясы; концентрацияның ауытқуы; жоғары концентрациялар; тасымалдау; қалалық көше каньоны.

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ЧИСЛЕННОЕ МОДЕЛИРОВАНИЕ РАСПРОСТРАНЕНИЕ ЗАГРЯЗНЯЮЩИХ ВЕЩЕСТВ В ЖИЛЫХ РАЙОНАХ

Аннотация. В данном исследовании проведено численное моделирование распределения загрязняющих веществ в уличном каньоне и влияния барьеров на этот процесс. Для решения этой задачи было использовано усредненное по Рейнольдсу уравнение Навье-Стокса. Для решения этой задачи была использована турбулентная модель DES, которая показала хорошие результаты для тестовой задачи. Для проверки математической модели и численного алгоритма была решена тестовая задача. Полученные численные результаты сравнивались с экспериментальными данными и результатами моделирования других авторов. После проверки математической модели и численного алгоритма была описана основная задача с

учетом процесса эмиссии загрязняющих веществ между домами, использующими различные высоты барьера. В качестве вычислительной площади была взята модель уличного каньона с соотношением сторон, которое колебалось от 0,05 м до 0,2 м. Как показывает численное моделирование, наличие барьеров приводит к появлению дополнительного вихря в пространстве между объектами, который увеличивается по мере увеличения их высоты. В результате можно наблюдать, что большинство загрязняющих веществ попадает в ловушку между ними. В ходе различных исследований было выявлено, что наличие барьеров вдоль дорог снижает концентрацию вредных веществ в воздухе. Поэтому при использовании травяного барьера высотой 0,1 м значение концентрации попадает в сечение x=0,05 м более чем в 1,5 раза по сравнению с без использования барьеров. Таким образом, можно сказать, что барьеры обеспечивают хорошую фильтрацию загрязненного воздуха, что пагубно сказывается на окружающей среде и здоровье человека.

Ключевые слова:загрязнение воздуха; дисперсия загрязняющих веществ; колебания концентрации; высокие концентрации; транспорт; городской уличный каньон.

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