Algerian Journal of Environmental Science and Technology
December edition. Vol.7. Nº4. (2021)
ISSN : 2437-1114
www.aljest.org

Evaluation and prediction of the effects of the dispersion of (VOCs) on the population in urban air using ANSYS CFX

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ARTICLE INFO

Article History:

Received ***:30/01/2020***
Accepted ***:01/07/2020***

***Key Words*:**

Benzene;
CFD simulation;
Dispersion;
Exhaust gas;
Motor vehicles;
ANSYS CFX.

ABSTRACT/RESUME

Abstract: *Indoor-outdoor environments are polluted by volatile organic compounds (VOCs), mainly benzene, toluene, ethylbenzene and the three isomers ortho, meta and para-xylene, commonly known as BTEX. Motor vehicles are the main source of these compounds. In this regard, we propose to study the simulation of the dispersion of benzene, emitted by the exhaust gases of a vehicle in a (3D) medium, in order to predict the concentration of the polluting gas and the different physical dispersion parameters as a function the distance from the emission source of the vehicle to the location of the study and the height of the buildings. In our work, CFD simulations were carried out using the k-ε turbulence model provided by the commercial code ANSYS-CFX. The results showed that whenever the source of pollution approaches the urban environment, pollution remains high in urban areas, which affects the well-being of the population.*

I. Introduction

The use of chemicals of organic or mineral origin presents a problem of toxicology on environment [1]. Volatile Organic Compounds (VOCs) are considered chemical substances consisting of carbon chains or rings, also containing hydrogen at a vapor pressure of more than 0.27 kPa at 25 °C, except methane [2]. The impact of disturbances and pollution is mainly reflected [3] by respiratory diseases and cancers. The results of air pollution monitoring research revealed [4-5] that VOCs are considered among the major air pollutants. The estimation of VOCs in several samples has been submitted with particular precaution in recent years [6]. because of the direct and indirect effects of [7] VOCs on human health and the ecological system. The majority of VOCs are carcinogenic or suspected compounds, and others have harmful impacts [8-10]. BTEX [benzene, toluene, ethylbenzene and the three isomers of xylene (ortho, meta and para)] are a subclass of VOCs boiling in the range of 80-150 °C. Based on the physico-chemical properties of BTEX, these compounds are very volatile and very flammable. They have a low solubility (1.76 g / L in water and 0.4 g / L in air for Benzene at 25 °C) [11-12], and a high solubility in oils and in most organic solvents. The change in solubility of Benzene is proportional to the temperature [11]. They are easily accessible to microorganisms in dissolved form. BTEX is moderately adsorbed by the organic phase of the soil. Their value of octanol / water partition coefficient (log Koc) is between 2 and 4. If the value of the partition coefficient is greater than 1, this means that the substance is more easily soluble in fat than in water, while if this value is less than 1, the substance will be more soluble in water than in fat. Aromatic hydrocarbon substances are highly available in the environment by reason of natural sources, which includes algae and plankton, also anthropogenic sources of hydrocarbons; including household and industrial waste, biomass and wood, incomplete combustion of fuel oil and urban runoff [2]. The main problems of air pollution [5] due to car emissions, essential VOC in urban areas [10]. Road transport is considered the main source of several polluting elements [13]. The road traffic exhaust participate with 55% of non-methane hydrocarbons [14]. Studies carried out in an urban environment in Algiers have shown that the level of air pollution by BTEX varied from 1.1 to 26.8 µg / m^3 for benzene, 3.5 to 63.3 µg / m^3 for Toluene, 2 to 12 µg / m^3 for Ethylbenzene and 1.07 to 14.7 µg / m^3 for Xylenes. For this, the observation, modelling, management, evaluation and prediction of the effects of air pollution on health and the environment are essential for sustainable development, especially in large urban agglomerations.

From the previous discussion, it can be seen that the CFD has become a more accessible tool due to the continued progress of modeling studies and the rapid increase of computational resources. However, from the foregoing published literature it seems that the results are varied, confuses sometimes contradictory. Separated flows are significantly affected by the presence of walls, where the viscosity-affected regions have large gradients in the solution variables and accurate presentation of the near-wall region determines successful prediction of separated-reattachment turbulent flows. In addition, it is known that the results of CFD simulations [15] are very sensitive to a wide range of computational parameters such as turbulence constants, and the flow profiles of velocity and turbulence quantities.

The objective of our work is to implement new ways [1] of detecting the pollution by using CFD simulation of the flow and dispersion of a pollutant in a (3D) environment in an urban agglomeration by applying the Reynolds Average Naviers-Stocks approach (RANS) based on a turbulence model k-ε implemented in the code CFD (Computational Fluid Dynamics) by ANSYS CFX. The results of the simulations are presented in order to study the structure of the flow and the dispersion in the urban agglomerations.

II. Methodology

II.1. Hypotheses

More than 90% of the benzene present in the ambient air is emitted by car traffic [13] The values due to traffic (%) are presented in Table 1. In order to study the dispersion of the pollution [16], we chose the case of a source of benzene emission coming from an exhaust pipe of a vehicle in stopping position in an urban agglomeration. To do this, we proceeded to the realization of different architectures of buildings with change of position of the source of emission with respect to these and this in order to follow the phenomenon of dispersion of this pollutant according to the variations of the heights of the buildings. Other parameters of dispersion, such as [17] pressure and temperature, have also been studied in order to better interpret the results of the modeling. The geometries of the studied buildings are realized according to the current architecture of the Algerian cities and in particular the city of Medea. The maximum and minimum heights of the studied buildings were 18 and 12 m. the number of buildings taken into consideration is four. It was estimated that between these four buildings were sidewalks and a six and a half meter two lane road, with a total distance of 8 m between the two buildings. The direction of dispersion of the pollutants was taken in the same direction of the prevailing wind. The city of Medea is considered a mountainous city and the four buildings are located next to a mountain that traps the flow of pollution rejected by cars. The buildings are located on a plot of 7500 m^2. For the modeling of pollution of the gas of benzene, two cases have been assumed. In all cases, it was considered that the road was between buildings of the same height. In the first case, we change the position of the emission source. In the second case, the change applies to heights of buildings (12 m). Vehicle traffic on the various routes studied was assumed very crowded. The modeling of the benzene dispersion was studied in May in stable atmospheric conditions (sunny day, wind speed 3 m / s according to the standards of the sidi-mselem meteorological station, MEDEA), without photochemical reaction leading to its elimination or the formation of other secondary pollutants.

Table 1. *Emissions of some pollutants in Europe* [13].

Substance	**Total emission (million t)**	**Percentage due to traffic (%)**
Sulfur dioxide	1	7.4
Carbon monoxide	8.25	73.8
Benzene	0.043	90

II.2. Numerical sumilation

Ansys CFX code, based on Finite Volume Method (FVM), was used for the solution of the conservation equations that governing the problem (Navier-Stokes and turbulence quantities) for all of turbulence models used in this study. Calculation are performed using the k-ϵ model. A standard k-ϵ turbulence model employed for wall relation to form the kinetic energy values of turbulence and dissipation at the first point of the array that moves away from the wall [18].

The turbulent kinetic energy ***k*** (m^2/s^2) is defined as follows equation (1) [19]:

$$k = \frac{1}{2}\overline{u_i u_i} = \frac{1}{2}\left(\overline{u_1^2 + u_2^2 + u_3^2}\right) \qquad \textbf{(1)}$$

Where u_i floating speed component in direction i (m / s).

The dissipation rate ε of the kinetic energy k is calculated from the equation (2):

$$\varepsilon = v\, \overline{\frac{\partial u_i \partial u_i}{\partial x_j \partial x_j}} \quad \textbf{(2)}$$

With v Kinematic viscosity (m^2/s).
Transport equation of turbulent kinetic energy k is given by equation (3):

$$\underbrace{\frac{\partial}{\partial x_i}(\rho k \overline{U_i})}_{a} = \underbrace{\frac{\partial}{\partial x_j}\left[\left(\mu + \frac{\mu_t}{\sigma_k}\right)\frac{\partial k}{\partial x_j}\right]}_{b} + \underbrace{G_k}_{c} - \underbrace{\rho\varepsilon}_{d} \quad \textbf{(3)}$$

a : Convective term
b : Broadcast term
c : Production rate
d : Dissipation rate
With ρ Density (kg / m^3), k Turbulent kinetic energy (m^2/s^2), $\overline{Ui}$ Average speed component in direction i (m/s), μ: Dynamic viscosity (kg/m.s), μ_t Turbulent dynamic viscosity (kg/m.s),
Enables the turbulent viscosity μ_t to be found from equation (4) or its equivalent in terms of

$$\mu_t = \frac{C_\mu \rho k^2}{\varepsilon} \quad \textbf{(4)}$$

Equation (5) define transport equation of the dissipation rate of turbulent kinetic energy ε:

$$\frac{\partial}{\partial x_i}(\rho\varepsilon\overline{U_i}) = \frac{\partial}{\partial x_j}\left[\left(\mu + \frac{\mu_t}{\sigma_\varepsilon}\right)\frac{\partial \varepsilon}{\partial x_j}\right] + C_{1\varepsilon}\frac{\varepsilon}{k}(G_k) - C_{2\varepsilon}\rho\frac{\varepsilon^2}{k} \quad \textbf{(5)}$$

The production term G_k is given by equation (6):

$$G_k = -\rho\overline{u_i u_j}\frac{\partial \overline{U_j}}{\partial x_i} = \rho v_t\left(\frac{\partial \overline{U_i}}{\partial x_j} + \frac{\partial \overline{U_j}}{\partial x_i}\right)\frac{\partial \overline{U_i}}{\partial x_j} \quad \textbf{(6)}$$

The adaptation of the standard constants of the model given by [20] makes the equation system operational. They are combined in Table 2:

Table 2. *Values of the constants of the k-ε model.*

C_μ	$C_{1\varepsilon}$	$C_{2\varepsilon}$	σ_k	σ_ε
0.09	1.44	1.92	1	1.3

In all the numerical simulation the accuracy of the results were dependent on the turbulence models, the near-wall treatment (y^+) applied, convergence criteria, among other solver factors.

The wall y^+ is a non-dimensional distance similar to local Reynolds number. In the context of CFD, it is used to describe how coarse or fine a mesh is for a particular flow. It determines whether the influences in the wall-adjacent cells are laminar, transitional or turbulent, hence indicating the part of the turbulent boundary layer that is resolved (ANSY CFX). It is described as:

$$y^+ = \frac{u^* y}{v} \quad \textbf{(7)}$$

Where y is the height from the wall to the mid-point of the wall-adjacent cells, υ is the kinematic viscosity and u^* is the friction velocity.
The pre-processor ICEM associated with Ansys is used for the construction of the computational domain and grid generation. A Cartesian structured grid non-uniform in the tow direction X and Y is used. A special attention was paid to the generation, in particular near wall treatment. Due to network adaptation, this is a major step in validating the model for future analysis. A special attention was paid to the generation, in particular near wall treatment. Because the grid adaptation it is a major step in validating the model for future analysis. In all cases the choice of grid mesh configuration, with respect to the turbulence model selected, was based the value of the non dimensional distance from the wall y^+ calculated using equation (7). The grid was adjusted multiple times based on the y^+ values of near wall cells until the y^+ values were within the limiting range. After the first node near the wall, the mesh is refined to capture high gradient of velocity, pressure and turbulence quantities in the vicinity of the wall. For each turbulence model used, a grid independence study was carried to find the mesh that allows a compromise between desired accuracy and solution cost in time and memory. For this purpose, three mesh sizes of significantly different grid resolution has been tested for the k-ϵ model studied, named coarse, mean refined and dense mesh as detailed in table 3. For turbulence models that use wall functions equation (k-ε), the first cell is placed in the fully turbulent (log-law region) just after the buffer layer which satisfy the condition $y^+ \approx 30$.
A sample of convergence history is illustrated in Fig. 1:

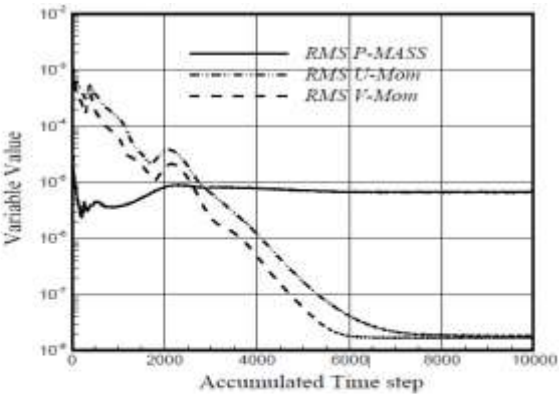

Figure 1. *Convergences.*

This research examines a potential application of a new configuration to predict the concentration and effects of air pollution, around of an urban agglomeration, generated by the exhaust pipe of a vehicle in a shutdown position in different places close to these buildings. Fig. 2 shows the configuration dimensions and conditions for the field of study, Fig. 3 shows the inputs and outputs for the field of study.

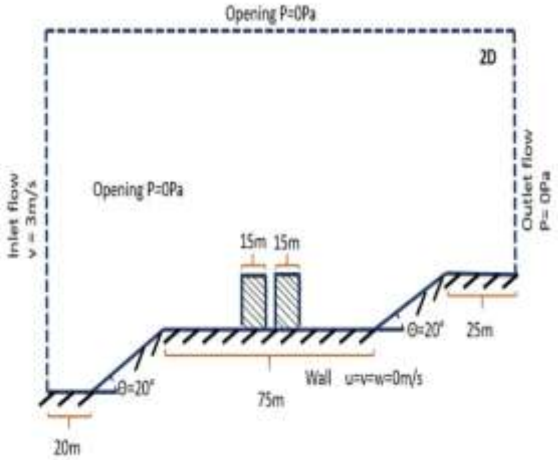

Figure 2. *Configuration dimensions and conditions.*

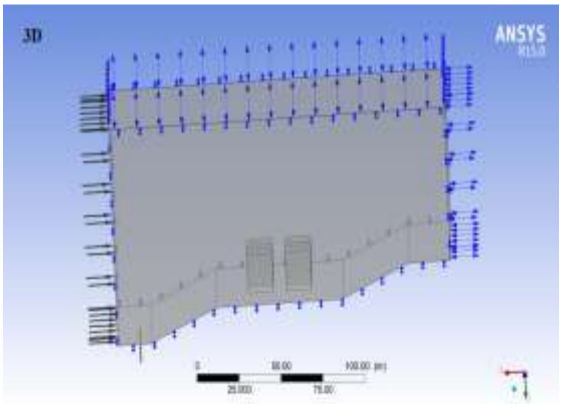

Figure 3. *The direction of the inputs and outputs of the domain to study.*

Fig. 4 shows the detail of the mesh of the geometry.

The entire domain was mainly composed of triangular cells. The parameters of the mesh are presented in Table 3:

Table 3. *The mesh parameters.*

Relevance center	**Sizing**	**Details**			
		Source of gaz dispersion in the middle of 4 buildings (H=18m)	**Source of gaz dispersion at 7 m from the facades of buildings (H= 18m)**	**Source of gas dispersion down-stream of buildings (H= 18m)**	**Source of dispersion in the middle of 4 buildings (H= 12m)**
Refined	Elements	185722	186648	188147	182256
	Nodes	35388	35515	35757	34761
Medium	Elements	59907	63115	63585	60376
	Nodes	11733	12247	12327	11792
Coarse	Elements	24488	27237	25859	25356
	Nodes	4824	5220	4950	4945

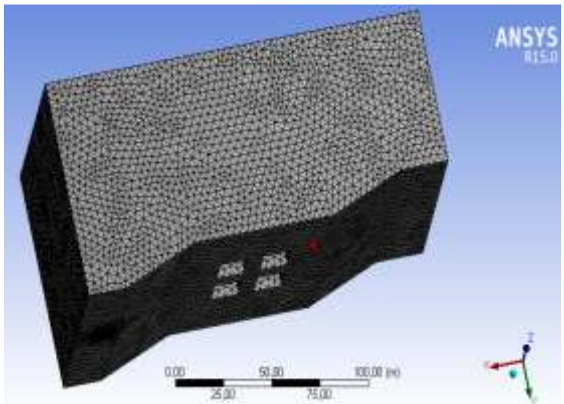

Figure 4. *Detail of the final mesh.*

II.3. Initial and boundary conditions

In the equations below, v: is the flow velocity vector field, C: is the concentration of polluting gas and Q: represents the flow, It should be noted that all the quantities of this equation are in SI units. Equation (8) define the initial condition, while equation (9), (10) and (11) defines boundary conditions, validated in the three directions, namely x, y and z.

$$C|_{t=0} = 0 \quad \textbf{(8)}$$

$$C|_{\text{pollution source}} = C^{sat} \quad \textbf{(9)}$$

$$Q|_{(\text{inlet})} = Q_i \quad \textbf{(10)}$$

$$v|_{\text{wall}} = 0 \quad \textbf{(11)}$$

III. Results and discussion

Four cases with different sources of pollution are simulated and analyzed, in the first three cases, the height of the building is 18m, that is to say, ground floor plus five floors, with the first case the source of pollution located between the four buildings , the second case, the source of pollution is distant with 7m of the facades of the two buildings and the third case the source of pollution is located on a plateau below the level of the four buildings, the fourth case the source of pollution located between the four buildings of 12m height ie ground floor plus three floors.

The parameters concerned in this study is the velocity in (m / s) and the volume fraction of benzene in the field of study. Simulation of the dispersion of the studied pollutant (C_6H_6) emitted at the exhaust pipe of a vehicle parked in the center of buildings maximum heights of 18 m, showed that the highest grades are concentrated at the bottom of buildings at about 5 m height. These high levels are due the emission source is surrounded by buildings that it brake, in the direction of the wind current. The dispersion of pollution at the level of buildings at the foot of the slope. Low concentrations are found near the slope Figs. 5, 6.

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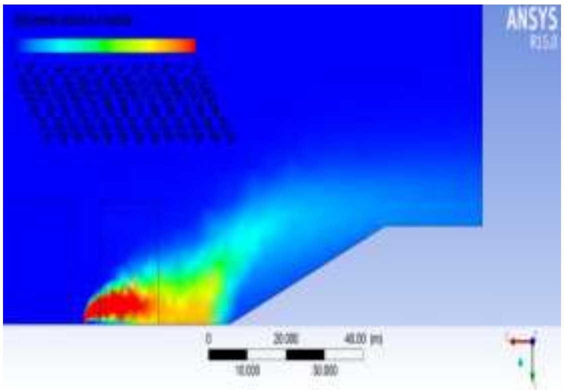

Figure 5. *Gas dispersion at the center of buildings H = 18m.*

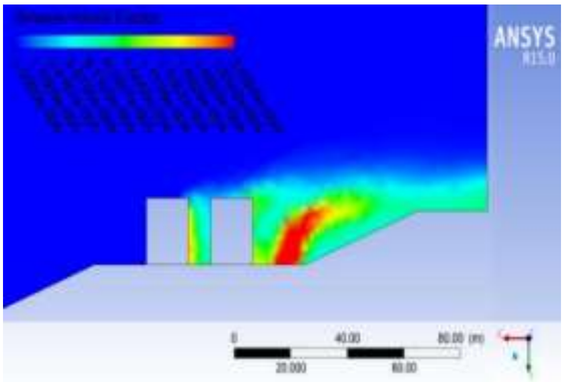

Figure 6. *Gas dispersion in the middle of buildings H = 18m.*

The study of the evolution of the exit velocity of the exhaust gases as a function of altitude has shown that the dispersion speed is high at buildings upstream of the source and decreases sharply at the foot of the slope which explains the low concentrations in the center and at the foot of the slope, (v between 2,5 and 3,12 m/s) Figs. 7, 8.

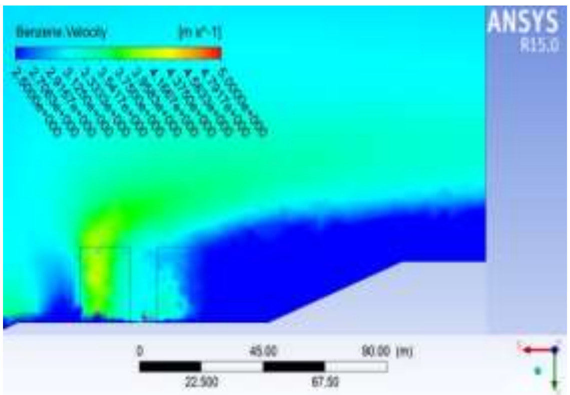

Figure 7. *Exhaust gas velocity at the center of buildings.*

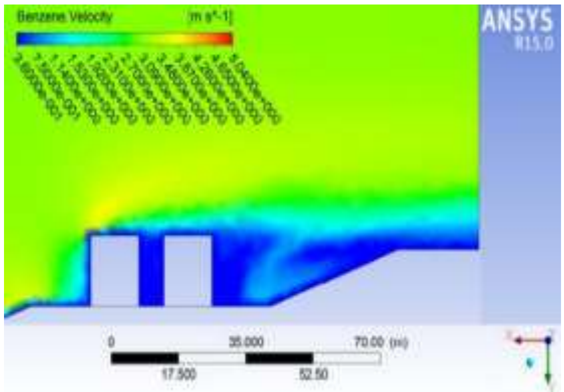

Figure 8. *Speed of gases in contact with buildings H = 18m.*

The study of the dispersion of benzene contained in the exhaust gases in the case where the source is located at the axis and 7 m upstream of the buildings, showed that the highest concentrations are located at the buildings that are close to the source emitting and in the lowest levels in buildings and at the foot of the embankment that have led to stagnation and slowing of drafts Figs. 9, 10.

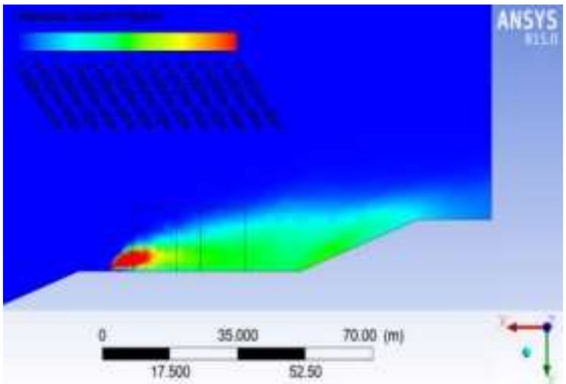

Figure 9. *Dispersion of gas at a distance of 7 m from the axis of the buildings.*

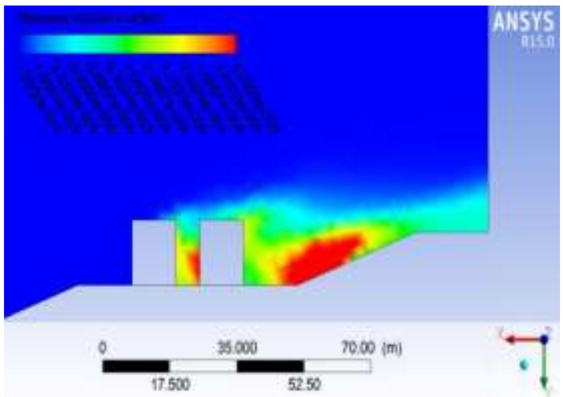

Figure 10. *Gas dispersion at 7 m from the building facades.*

The study of the evolution of the exit velocity of the benzene, contained in the exhaust gases, confirms the high concentrations at 7 m from the axis of the facades of the buildings, and between the two buildings that are close to the source of pollution, thanks to the decrease of the dispersion surface, which favors the increase of the speed Fig. 11. According to Figs. 11, 12 it is noted that the lowest speeds are downstream of buildings and at the foot of the slope.

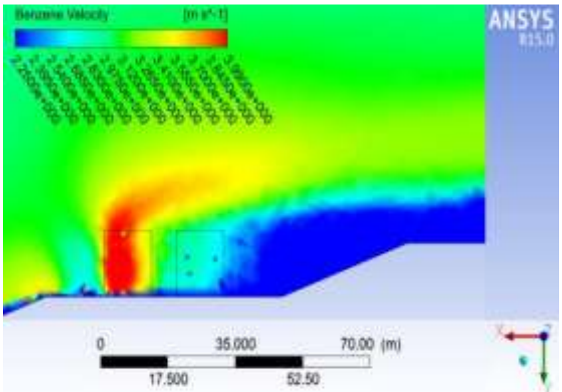

Figure 11. *Exhaust gas velocity at a distance of 7 m from the axis of the building.*

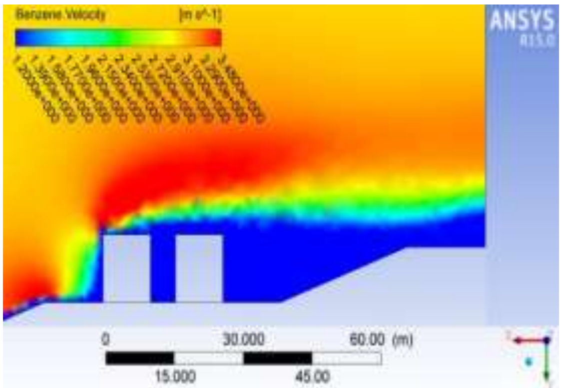

Figure 12. *Speed of benzene in contact with buildings.*

To better study the dispersion of benzene gas, it has been assumed that there is an emitting source located in another slope below the buildings. The chosen angle was identical to that which is downstream of the buildings. The study shows that the high concentrations fit the shape of the lower slope and then the soil. Pollution by benzene at the building level has almost reached the height of buildings and then decreases sharply at the upper slope due to the effect of air recirculation Figs. 13, 14.

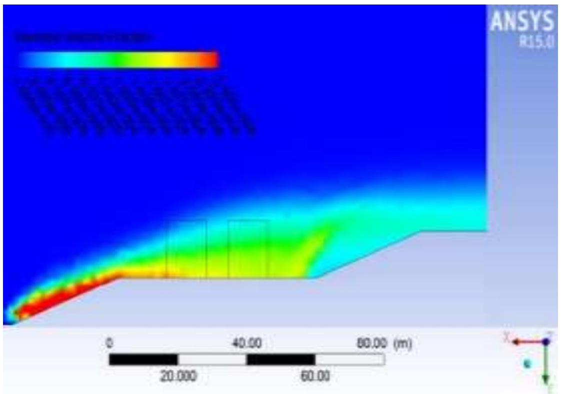

Figure 13. *Dispersion of gases at a source downstream from the axis of the buildings.*

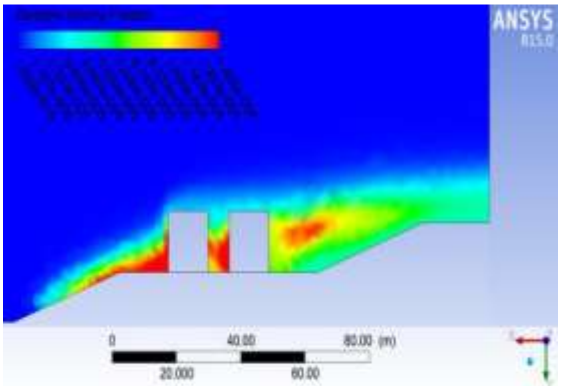

Figure 14. *Effect of gas dispersion on the source downstream of buildings.*

According to Figs. 15, 16 the exit velocity of the benzene contained in the exhaust gases clearly shows that the latter evolve in a homogeneous manner around the lower slope and the buildings hence the levels recorded which are due to the recirculation of the air at the level of the buildings. In consonance with Fig. 15, the increase in speed between the first two buildings due to the decrease of the dispersion surface.

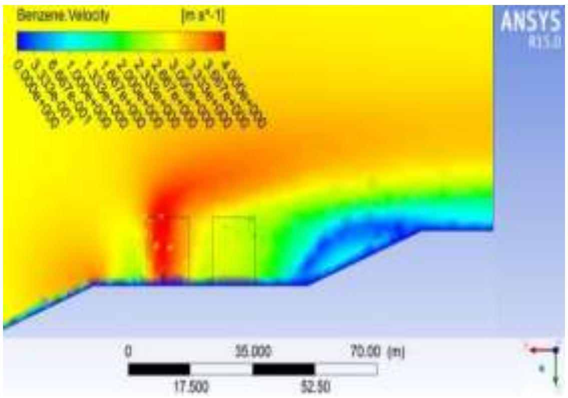

Figure 15. *Benzene velocity at a source below the axis of the building.*

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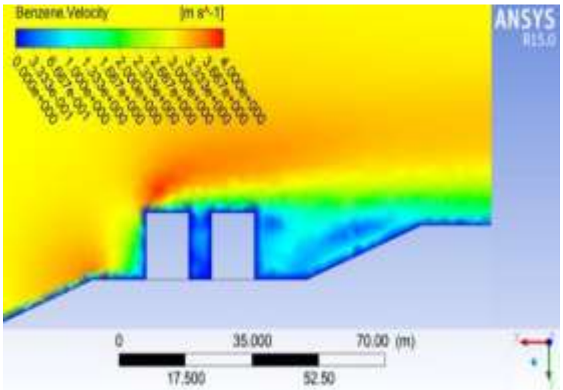

Figure 16. *The effect of Benzene speed during contact with buildings.*

In the case where the source of emission is in the center of the buildings of 12 m of height, the study of the dispersion showed a strong accumulation of the polluting gas (C_6H_6) near the upper slope because of the imprisonment and the braking effect by the buildings and the slope. In this case, almost all levels of buildings are affected by pollution Fig. 17 hence a negative impact on the population.

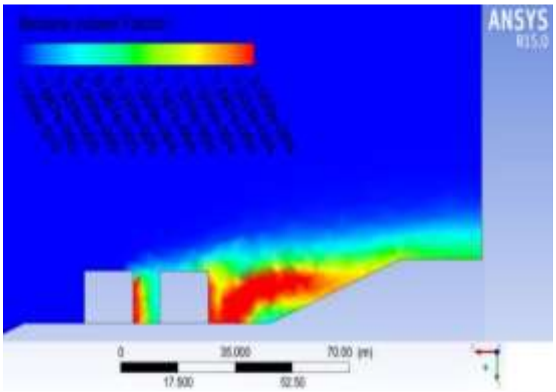

Figure 17. *Height effect of buildings H = 12 m on pollutant gas accumulation.*

The study of the evolution of the speed shows the effect of stagnation at the level of the heights of the buildings Fig. 18.

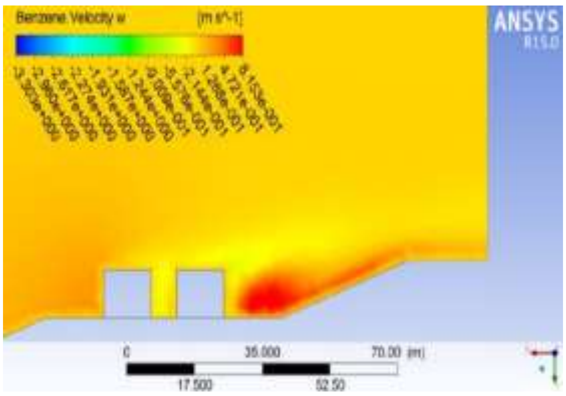

Figure 18. *Effect of the height of the building H = 12 m on the speed of dispersion of the gaseous pollutants.*

IV. Conclusion

According to the results obtained by the simulation of the dispersion of benzene contained in the exhaust gas at the level of the buildings located in a mountainous city, by the Commercial code ANSYS CFX. It has been shown that the geometry of buildings plays an important role in the phenomenon of transport of emitted gases (C_6H_6). Note that when the height of the building is large (H = 18 m), the gases emitted are not trapped between the building and the slope, which is beneficial and favorable to have a good dispersion. In this case, the heights of the buildings are considered as an obstacle to the air circulation, on the other hand, when the height of the building is a little low (H = 12 m). The pollutant will be trapped between the building and the slope, which will cause gas accumulation and poor dispersion, that affects the health of the population.

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Please cite this Article as:
Ibrir A., Kerchich Y., Hadidi N., Rebhi R., *Evaluation and prediction of the effects of the dispersion of (VOCs) on the population in urban air using ANSYS CFX,* **Algerian J. Env. Sc. Technology**, ***7*:4 (2021) 2135-2142**