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Modeling and Analysis of NO_x and O_3 in a Street Canyon

Merah Aissa[1,2*], Noureddine Abdelkader[2]

[1]Centre for Scientific and Technical Research in Physico-Chemical Analyzes, BP 384, Seat ex-Pasna Zone Industrielle, Bou-Ismail PO.Box-42004, Tipaza, Algeria
[2]Laboratory of Applied Mechanics LMA, Oran University of Science and Technology, Mohamed Boudiaf, Algeria

ABSTRACT

This study numerically investigates reactive pollutants (NO, NO_2 and O_3) flow and dispersion in a 3D street canyon in time and space, by using a CFD (computational fluid dynamics) code (ANSYS-CFX). An area source (sub-domains) for medium emissions of NO_x was considered in the presence of background O_3 concentration, with an ambient wind perpendicular to the along-canyon direction. Spatial and temporal variation of pollutants within the canyon was calculated to be significant. It was found that NO and NO_2 concentrations were higher at the upwind buildings (at lower levels near the street bottom) than near the downwind buildings, the largest concentrations of O_3 were observed towards the canyons' windward wall as O_3-rich air is brought into the canyon.

Keywords: ANSYS-CFX, NOx, O_3, Reactive pollutants, Street canyon

INTRODUCTION

Traffic emission is becoming a major source of air pollution in the urban environment with relatively densely packed buildings flanking narrow streets and continuous increase in motor vehicles. Streets are one of the most important urban elements, where population and traffic density are relatively high [1,2] and human exposure to hazardous substances is expected to significantly increase. Due to the very short distances between sources and receptors, only very fast chemical reactions have a significant influence on the measured concentrations within street canyons [3,4]. For this reason, most traffic-related pollutants (e.g., CO and hydrocarbons) can be considered as practically inert species within these distances. This is not the case either for NO_2; which dissociates extremely fast in the presence of light, or for NO, which also reacts very fast with O_3 [5] The time scales of these chemical reactions are of the order of 10 of seconds, thus comparable with residence times of the pollutants in a street canyon.

The chemical composition of the atmosphere has been used as important reference information to help policy-makers define effective emission reduction policies. There are literally thousands of chemical compounds, undergoing an even larger number of chemical reactions in the atmosphere. Because of the current limited computing power, the photochemical models are unable to include all the atmospheric chemical species and reactions simultaneously. Therefore, simplified, or the most representative, chemical mechanisms are introduced into photochemical models to provide a computationally viable means of representing what is understood about the chemical dynamics of trace compounds in street canyons. The CFD modeling approach as a way to understand street canyon flow and dispersion has become powerful and comprehensive with recent advances in computing power, numerical method/algorithm [6,7] and turbulence parameterization [8].

MATERIALS AND METHODS

Numerical simulations

Computational domain of street

The street canyon was chosen for the study, is one-way street with a length of 95 m (and 10 m of width). This street has about 19 building with heights varying between 3 m and 18 m. The computational domain size is 95 m × 16 m × 21 m (Figure 1a). The emission sources considered in this study are sub-domains (volume sources), created along the street in x direction (11 sub-domains or cars), with size of 3.5 m × 2 m × 1.48 m (Figure 1b).

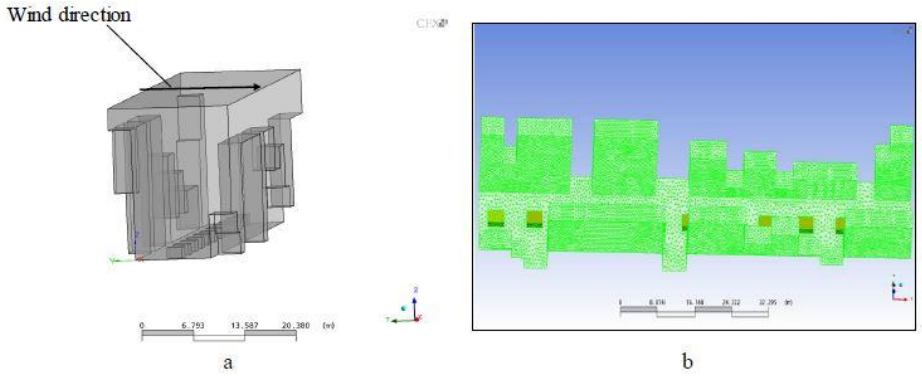

Figure 1: (a) The complete computational domain, (b) Surface mesh elements

Model description and chemical reactions

The CFD model chosen for this study (ANSYS-CFX) is based on the k-ε turbulence model to consider the chemical reaction and the transport of reactive pollutants within a street canyon. The reactive gases considered were NO and NO_2 emitted into the canyon by traffic against a background of ozone. The standard *k-ε* turbulence model governing equations expressed as (Table 1) [9]. The continuity Equation:

$$\frac{\partial U_i}{\partial x_i} = 0 \tag{1}$$

The momentum Equation:

$$\frac{\partial U_i}{\partial t} + U_j \frac{\partial U_i}{\partial x_i} = -\frac{1}{\rho}\frac{\partial \bar{p}}{\partial x_i} + \frac{\partial}{\partial x_j}\left(\upsilon \frac{\partial U_i}{\partial x_j} - \overline{u_i' u_j'}\right) \tag{2}$$

Where, *k* and *ε* transport equations in the standard *k-ε* model:

$$\frac{\partial k}{\partial t} + \vec{V}\vec{grad}k = div(\frac{\upsilon_t}{\sigma_k}\vec{grad}k) + P - \varepsilon \tag{3}$$

$$\frac{\partial \varepsilon}{\partial t} + \vec{V}\vec{grad}\varepsilon = div\left(\frac{\upsilon_t}{\sigma_\varepsilon}\vec{grad}\varepsilon\right) + \frac{\varepsilon}{k}\left(C_{\varepsilon_1}P - C_{\varepsilon_2}\varepsilon\right) \tag{4}$$

Where, *k* is the turbulent kinetic energy; *ε* denotes the turbulent dissipation rate. *P*: Production of *k*, *ε*: Dissipation of *k*.
Where,

$$\upsilon_t = C_\mu \frac{k^2}{\varepsilon};\ P = 2\upsilon_t S_{ij} S_{ij};\ \overline{u_i' u_j'} = -2\upsilon_t S_{ij} + \frac{2}{3}k\delta_{ij};\ S_{ij} = \frac{1}{2}\left[\frac{\partial U_i}{\partial x_j} + \frac{\partial U_j}{\partial x_i}\right]$$

Table 1: The constants for *k-ε* turbulence model

C_μ	σ_k	σ_ε	C_{ε_1}	C_{ε_2}
0.09	1	1.3	1.44	1.92

Pollutant concentration is calculated with the convective-diffusion Equation:

$$\frac{\partial C_i}{\partial t} + U_j \frac{\partial C_i}{\partial x_j} = \frac{\partial}{\partial x_j}\left(K_t \frac{\partial C_i}{\partial x_j}\right) + S_i \tag{5}$$

Where, C_i denotes the pollutant concentration, K_t is the eddy diffusivity coefficient and S_i represents all sources and sinks terms. The chemical reactions considered are:

NO_2+sunlight (λ<420 nm) → NO+(O^{3p})	(r_0)
(O^{3p})+O_2+M → O_3+M	(r_1)
O_3+NO → NO_2+O_2	(r_2)

M represents a molecule (N_2 or O_2 or another third molecule)

The kinetic rate constant (Arrhenius equation) for the reactions r_1 and r_2 is (Table 2):

$$k(T) = A \times T^{\beta} \, exp\left(\frac{-E_a}{R \times T}\right) \tag{6}$$

Where, A is a pre-exponential factor, β is the temperature exponent, R is the universal gas constant, T is the temperature, and E_a is the activation energy.

Table 2: The parameters for the reactions r_1 and r_2

Reaction	A	E_a	β
r_1	6.10^{-34}	0.0	-2.3
r_2	2.10^{-12}	2.782	0.0

The photolysis rate for the reaction r_0 calculated using the expression [10]:

$$J_{NO_2} = 8.14 \times 10^{-3} \times \left[0.97694 + 8.14 \times 10^{-4} \times (T - 273.15) + 4.5173 \times 10^{-6} \times (T - 273.15)^2\right] \tag{7}$$

Where, T is in K and the unit of J_{NO2} is s^{-1}.

Boundaries and initials conditions

The vehicles were assumed to emit NO of 18.3 µg/m^{3}s (90% of NO_x), and 2.03 µg/m^{3}s of NO_2 (10% of NO_x) for each car [11]. A background ozone concentration of 70 µg/m^3 (as mass fraction f_{O3}=5.8 x 10^{-8}) was then set for the entire domain and the Initial values of mass fraction of NO_2 and NO are f_{NO2}=2.025 x 10^{-8} (24 µg/m^3), f_{NO}=1.02 x 10^{-8} (12 µg/m^3) respectively. At the inflow, the wind velocity assumed as profile (perpendicular to the street) [12] and is given by:

$$U(z) = U_{ref}\left(\frac{z}{z_{ref}}\right)^{\alpha} \tag{8}$$

Where, z_{ref}, U_{ref} are the reference height (10 m) and reference velocity (1.5 m/s), respectively, α is the power law exponent (0.299), (Figure 2). The pressure and temperature were specified as 1 atm and 25°C, respectively.

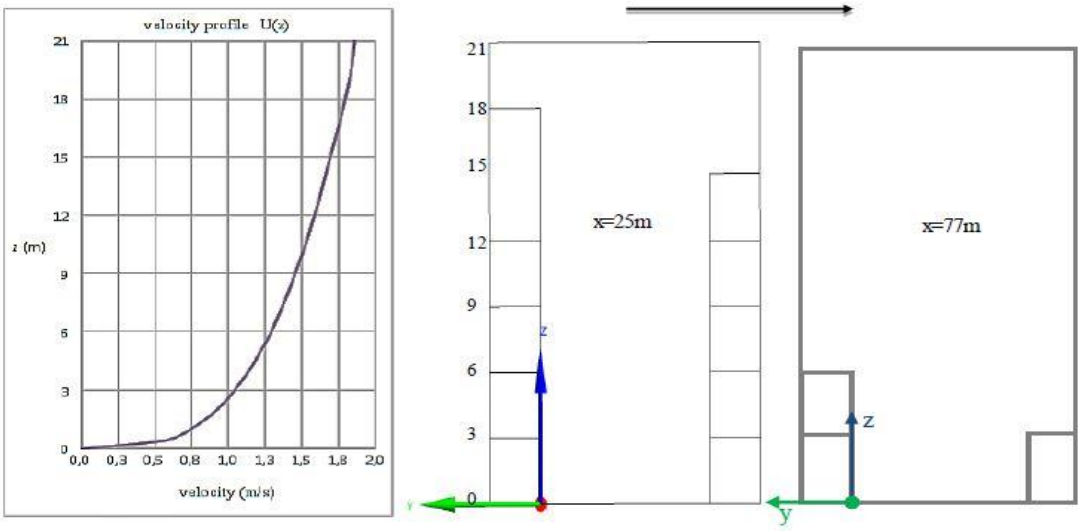

Figure 2: Velocity profile plot at inflow boundary (left), wind direction perpendicular to the street on x-y plane (at x=25 and 77 m positions) (right)

RESULTS AND DISCUSSION

The results presented in Figure 3 show the NO and NO_2 concentration fields and reflects the existence of a vortex in the street canyon for the both positions (x=25 m, x=77 m), the magnitude of pollutant concentrations on the leeward side is larger than the windward side buildings (near the corner of the downwind buildings), due the primary vortex recirculates emitted pollutants therein, and the peak values of NO and NO_2 are 1.82×10^{-7} kg/m^3, 2.42×10^{-7} kg/m^3 at x=77 m and 2.4×10^{-7} kg/m^3, 2.5×10^{-7} kg/m^3 at x=25 m, respectively.

On the other hand, there is a formation of NO_2 due to the reactions between O_3 and NO and thus, NO_2 dispersed more significantly than NO [13]. The O_3 concentration is high (6.88×10^{-8} kg/m^3) near the upper downwind region of the street canyon where ambient ozone intrudes into the canyon [14] and Most exchange takes place near the windward wall where air is entering the canyon from above roof level and pollutants are able to escape [13].

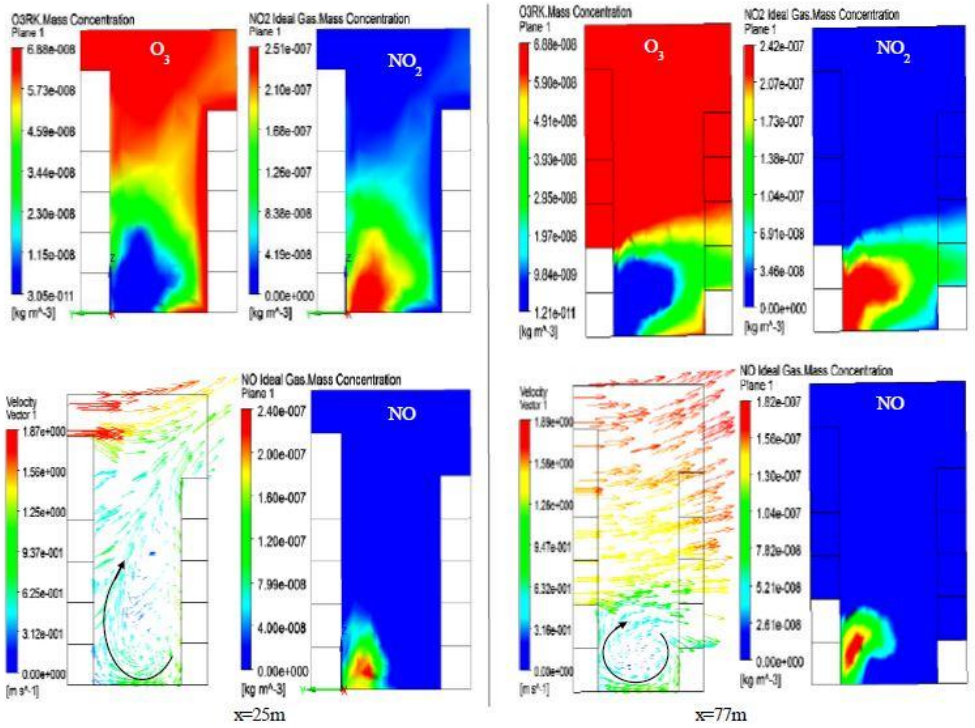

Figure 3: O_3, NO_2, NO concentrations and velocity vectors on y-z plane at x=25 m and x=77 m

The Figure 4A presents the correlation between the reactive pollutants for the complete domain (Where the wind direction perpendicular to the street), In Figure 4A (NO_2/NO graph), it is observed that there is a proportional increase between the concentrations of NO and NO_2, above the 1.5×10^{-7} kg/m^3 of NO_2, this is explain by the increasing of the NO and NO_2 concentrations in leeward wall and in the near the street bottom (in the corner). Under the 1.5×10^{-7} kg/m^3 of NO_2, the NO concentration is nearly to zero, because the dispersion of NO is limited than NO_2. In the Figure 4A (O_3/NO_2 graph) it can be explained the increasing of the NO_2 concentration with decreasing of O_3 concentration by the consummation of O_3 (by NO) leads to a significant increase of the NO_2 [15].

Last graph (O_3/NO) in Figure 4A shows that is a disparity in the variation of O_3 concentration with NO (a similar of NO With O_3) this is explained by the reaction between them near the increasing of NO (in the street corner), and in the regions where the high concentration of O_3, the NO Concentration is very low (upper downwind region and windward wall). It is very clear that there is a similarity between the graphs of Figure 4A (This study-wind perpendicular to the street) and Figure 4B (Merah et al., wind parallel to the street), this means that the correlation between the pollutants remained almost unchanged, despite a change of wind direction, and thus changed the places of exchange and interaction. Because this correlation reflects the reactions between these pollutants [16,17].

Transient simulation (wind perpendicular to the street)

In this part, in the beginning, we have simulated a steady state with presence of a background of ozone, but without the emission of NO_x, The results from this simulation were used as the initial values file for the transient simulation (90 sec) where the NO_x emission has been started. The results of the transient case are presented in the Figure 5, which shows the variation of average concentration of O_3, NO_2 and NO with time for different levels (at x=25 m and 77 m). Firstly, We can observe that the average concentration of NO_2 increases rapidly in the early time in the lower layers and then remains almost constant after 40 sec, and that the concentration decreases as altitude increased (to be almost zero at 12 and 18 m), so for example (at x=25 m) decreases by 25% at 4 m and 60% at 6 m, but for the case of x=77 m where the building heights are 6-3 m, the NO_2 average concentration at the level of 4 m higher than at the level of 2 m, it is due to the escape of pollutants (NO_2) is significantly above the windward building (3 m) in Figure 3.

Secondly, the reverse is the case for ozone, the average concentration of ozone decreases with a time lag in the lower layers, from the maximum

value 6.88×10^{-8} kg/m^3 to the lowest values, then remain nearly constant the end of time (after 60 sec). This is associated with NO emission and its dispersion, especially at the lower levels. Therefore, we have noted that ozone decreased by 78% at 2 m, 66% at 4 m and by 36% at 6 m, But at higher levels remained generally steady at the maximum value. Also for x=77 m note that O_3 average concentration at level of 2 m is higher than at level of 4 m, due to the same cause as NO_2 (noted above).

Finally, the average concentration of NO increases with time in the lower layers 2-4 m near the ground, due to the continued emitted from the source, and it takes time to transport to the high levels. for example, for x=25 m, reached 1.45×10^{-7} kg/m^3 at 2 m in 90 sec, also observed that the concentrations of NO for x=25 m is generally greater than for x=77 m, this due to its consumption by ozone is significantly there, It also becomes non-existent in the upper levels.

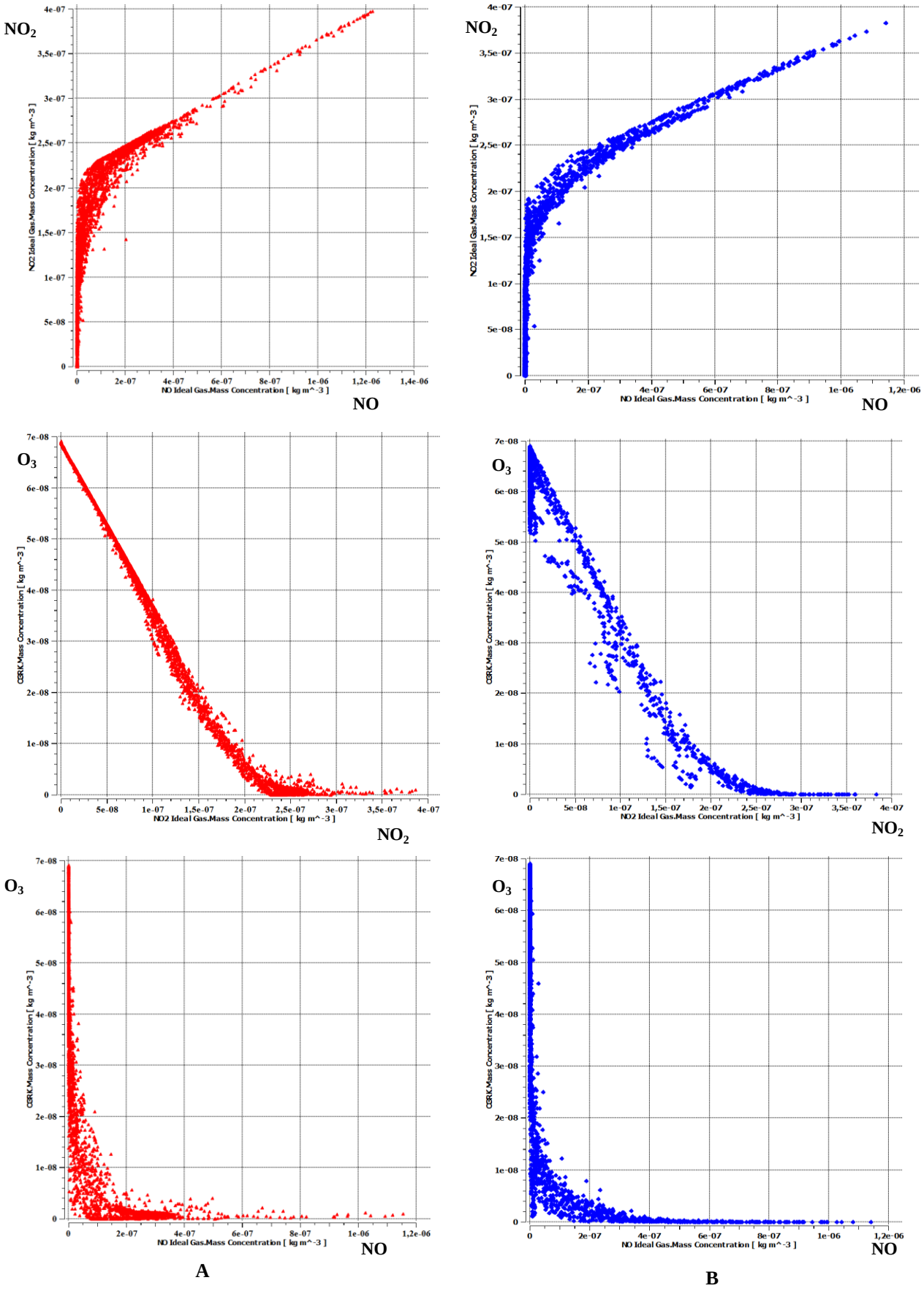

Figure 4: Domain average concentrations correlation: NO_2 with NO, O_3 with NO_2, and O_3 with NO A-This study (wind perpendicular to the street), B-Merah et al., 2016 (wind parallel to the street)

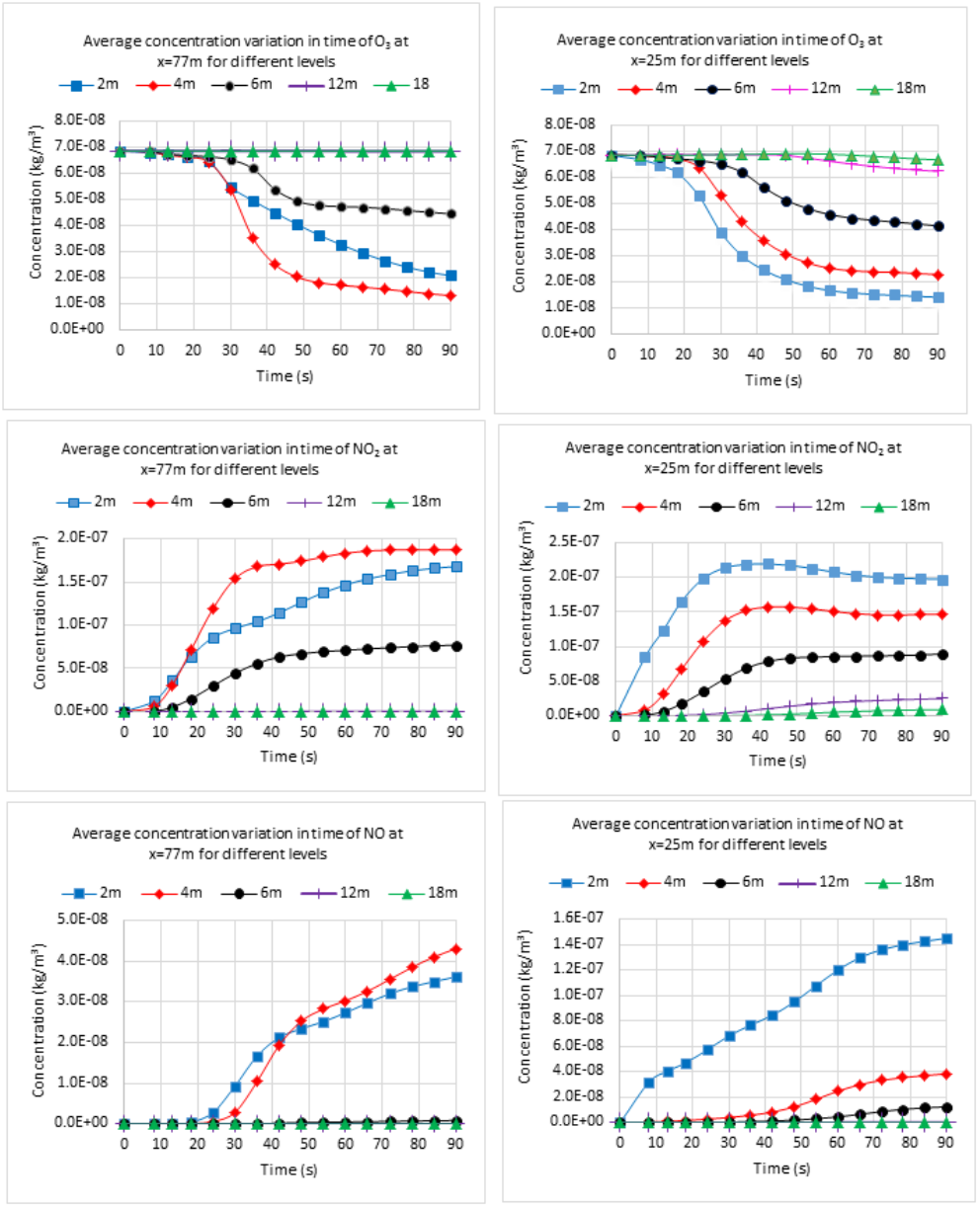

Figure 5: Average concentration variation in time of O_3, NO_2 and NO for different levels at: (left) x=77 m, (right) x=25 m

CONCLUSION

The results indicated that the wind perpendicular to the street leads to accumulation of pollutants inside the street canyon with a different degree depending on buildings height, as the height of buildings increases, the pollution level increases, that is, the concentration (NO, NO_2) is higher near the downwind building than near the upwind building, due the vortex recirculates emitted pollutants therein. The highest within-canyon concentrations of O_3 were observed near the upper downwind region of the street canyon where ambient ozone intrudes into the canyon. It is interesting to observe that under the increasing buildings height the amount of intrusion of ambient ozone into the canyon has been increased. It is indicated that increment of building height encourages the accumulation of ozone. On the other hand when compared this study with (Merah et al.,) it found that the correlation between the pollutants remained almost unchanged, despite a change of wind direction, and thus changed the places of exchange and interaction. Because this correlation reflects the reactions between these pollutants.

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REFERENCES

[1] P. Kastner-Klein, P.J. Plate, *Atmos. Environ*., **1999**, 33, 3937-3979.
[2] R.N. Meroney, M. Pavageau, *J. Wind. Eng. Ind. Aerodyn*., **1996**, 62, 37-56.
[3] J. Baker, L. Walker Helen, X. Cai, *Atmos. Environ*., **2004**, 38, 6883-6892.
[4] M.W. Rotach, *Atmos. Environ*., **1995**, 29, 1473-1486.
[5] P. Finn, B. Ruwim, H. Ole, V. Elisabetta, *Sci. Total. Environ*., **1996**, 189/190,409-415.

[6] T.R. Oke, *Energ. Bldg*., **1988**, 11, 103-131.
[7] W.C. Cheng, L. Chun-Ho, D.Y.C. Leung, *Atmos. Environ*., **2009**, 43, 3682-3690.
[8] B. Jong-Jin, K. Jae-Jin, *J. Appl. Meteo*., **1999**, 38(11), 1576-1589.
[9] J.F. Sini, S. Anquetin, G. Mestayer, *Atmos. Environ*., **1996**, 30, 2659-2677.
[10] J.J. Baik, J.J. Kim, *Atmos. Environ*., **2002**, 36, 527-536.
[11] A. Merah, A. Noureddine, M. Abidat, *Der. Pharma. Chemica*., **2016**, 8, 418-424.
[12] T. Yoshihide, M. Akashi, Y. Ryuichiro, K. Hiroto, N. Tsuyoshi, Y. Masaru, S.T Shirasawa, *J. Wind. Eng. Ind. Aerod*., **2008**, 96, 1749-1761.
[13] V.B. Bright, W.J. Bloss, X. Cai, *Atmos. Environ*., **2013**, 68, 127-142.
[14] J.J. Baik, Y.S. Kang, J.J. Kim, *Atmos. Environ.*, **2007**, 41, 934-949.
[15] A.G. Triantafyllou, S. Zoras, V. Evagelopoulos, S. Garas, C. Diamantopoulos, *Global. NEST. J.* **2008**, 10, 161-168.
[16] M. Yucong, L. Shuhua, Z. Yijia, W. Shu, L. Yuan, *J. Adven. Meteo*., **2014**, 458671.
[17] G.T. Johnson, L.J. Hunter, *Atmos. Environ*., **1999**, 33, 3991-3999.