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Atmospheric Chemistry and Physics Discussions

Interactive comment on "CFD Modeling of Reactive Pollutants Dispersion in Simplified Urban Configurations with Different Chemical Mechanisms" *by* Beatriz Sanchez et al.

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Thank you for your appraisal of the manuscript and your comments for improving it. In regards to the information which was rather confusing, we have enhanced the comprehension. Particularly, we have clarified the methodology used and highlighted the main results from this work.

The responses to the SPECIFIC COMMENTS are described in the following lines and the corresponding changes in the manuscript have been highlighted in blue in the PDF file:

Abstract. *Overall I found the abstract a little bit confused. Several information are*

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mixed without a proper organization. I suggest the authors to introduce the problem, then discuss the methodology in a schematic way and then main results.

This section has been re-organized and modified the confused sentences according to your comments. Please see this section in the PDF file.

***Introduction**. Please check throughout the paper that NOx, NO2 etc. have been defined before using chemical formula. Overall also the introduction is slightly confused. The same concepts are repeated throughout the section. At the end please underline the structure and the original contribution of the paper.*

This section has been re-written according to your comments. Please see the PDF file.

How did you estimate "a factor of 2"?

This is referred to as the computational time required to carry out the simulation with the complex chemical scheme implies more than twice the time demanded with the use of the photostationary steady state. This has been clarified in the revised manuscript, please see the PDF file (Page 3, lines 17-19).

***Chemical Scheme used**. Please introduce the scheme otherwise it is not easy to understand. RACM? - Reduced to 25 reactions with respect to?*

The reduced complex chemical scheme used in this work consists of 23 chemical species and 25 chemical reactions. This chemical scheme was developed from the Regional Atmospheric Chemistry Mechanism (RACM) with 77 species and 237 reactions. Thus, the computational time of simulating the reactive pollutant with the reduced mechanism was also reduced.

The chemical scheme has been introduced in order to understand it easily. Please see the PDF file (Page 3, lines 27-29; Page 4, lines 4-12).

***Simulation Setup**. Overall also this section is hard to follow.*

This section has been modified and re-structured as per your recommendations. Please read this section in the PDF file.

It is not clear why two so close wind velocities have been chosen. They are both calm conditions. If the results achieved are different based on the velocity, this should be discussed in terms of flow regime in the streets and turbulence.

The reference velocity (u_τ) used in the manuscript represent the friction velocity in order to compute the pressure gradient imposed on cyclic boundary conditions. For u_τ=0.22 m s^{-1} the corresponding wind speeds at 1.5H are 1.9 m s^{-1} and 1.5 m s^{-1} in the 2D and 3D geometries respectively, and the double for the u_τ=0.45 case, so differences are significant in terms of wind speed at 1.5H.

Wind speed and turbulence are proportional to u_τ and u_τ^2 respectively because thermal effects were not taken into account. Therefore, the flow regime in the streets is the same in both cases.

Some comments have been included in the manuscript in order to clarify this issue. Please see the PDF file (Page 6, lines 8-9).

How did you estimate 930 vehicles?

930 vehicles per hour can be representative of medium traffic (Baker et al., 2004). In this way, we have used the same emission source rates (S_{NO} and S_{NO_2}) considered in Baker et al. (2004). Therefore, whether the emission source of NOx is around 130 µg $m^{-1}s^{-1}$ ($S_{NO_x} = S_{NO} + S_{NO_2}$) and the NOx emission source per vehicle is around 0.5 g km^{-1} (Baker et al., 2004 and Baik et al.,2007). veh $s^{-1} = 130\,\mu g\,m^{-1}\,s^{-1}\frac{veh}{0.5\cdot10^3\mu g\,m^{-1}}$

CFD Model Evaluation. *I suggest also to validate flow and turbulence obtained from CFD and not only concentration at few points.*

Flow and turbulence corresponding to simulations with the 3D set up and the same CFD model were already validated in other work (Santiago et al., 2008). The flow and turbulence in the array of cubic obstacles has been evaluated using the DNS model results. Vertical profiles of the horizontally averaged wind speed, turbulent kinetic energy and Reynolds shear stress were compared as in Santiago et al. (2008). Similar profiles were obtained for both turbulence models (not shown in the manuscript).

Did the authors perform any sensitivity test of the grid and domain size?

In both geometries, we carried out a mesh independence test with a finer grid resolution. In the 2D geometry, we tested two grid resolutions: 0.5 m and 1 m in all directions. The vertical profiles of wind speed and turbulent kinetic energy from each mesh were compared with each other. The obtained results were equivalent and we therefore selected the grid resolution of 1 m. The vertical profile of the spatial average of turbulent kinetic energy is shown in Fig. 1. For the 3D geometry, the grid resolutions were: 0.5 m and 1 m in all directions. The wind speed and turbulence from each mesh resolution were compared and they showed the same results (Fig. 2). This is not shown in the manuscript, please see the attached figures.

As for the domain size, the height of the top was selected based on the results obtained in Coceal et al. (2006). They evaluated the effect of several domain heights concluding that 4H is a good assumption.

We have included some remarks about the sensitivity tests and added the reference in the manuscript. Please see in the PDF file (Page 6, lines 1-5).

Remarks should be added about other turbulence modelling, such as the RSM, LES.

Some comments about turbulence modeling have been added (Page 5, lines 11-14):

The CFD model used is based on the Reynolds-averaged Navier-Stokes equations (RANS) with a k-ε turbulence model. This model allows to evaluate the effect of several parameters using a wide set of simulations within a reasonable CPU time. The turbulence can be solved more accurately by other models such as Large Eddy Simulation or Direct Numerical Simulation, however the CPU load increases considerably and it would limit the number of simulations.

Results. *Discuss also the physical processes for 2d and 3d geometries and discuss throughout the text and in the conclusions also the differences between 2d and 3d geometries. It is not clear if one introduce more errors simplifying the geometry or the chemical reactions.*

The differences between the processes in the 2D and 3D geometries were not addressed here because we just focused on evaluating whether the effects of including chemical reactions led to the same conclusions in different types of geometries. Moreover, we would like to stress that the 2D is not considered a simplification of the 3D, rather a different type of urban structure.

In the course of this work, we have tried to understand how the behavior of a reactive pollutant differs from that of the non-reactive pollutant in each geometry. From the results, we have concluded that under some atmospheric conditions the difference between the chemical scenarios could be important in both geometries, regardless of the type of the geometries used in this study.

This approach has been modified in the revised manuscript in order to clarify the confused information. Please see PDF file.

It is recognised that 3d geometries lead to corner vortices which should improve the

dispersion from the streets. Please adjust and add a reference. Also the sentence 'Therefore, the residence time of each reactive compound within street is determined by building configurations and wind speed' is not clear since this is true both for 2d and 3d. - Pag. 9 Line 18. Domains? Do you mean in 2d and 3d geometries?

This has been clarified in the PDF file (Page 9, lines 5-9).

It is not strictly true that the concentration of non-reactive pollutant is inversely proportional to wind speed. It is true in flat terrain, but in the streets it may depend on other variables. Please add a reference.

Under the assumptions considered in this work, the concentration of non-reactive pollutant is inversely proportional to wind speed as shown in Parra et al. (2010). That is due to the fact that we are not including any processes that break this linearity such as thermal effects, pollutant deposition or turbulence induced by traffic.

Please also note the supplement to this comment:
http://www.atmos-chem-phys-discuss.net/acp-2016-202/acp-2016-202-AC2-supplement.pdf

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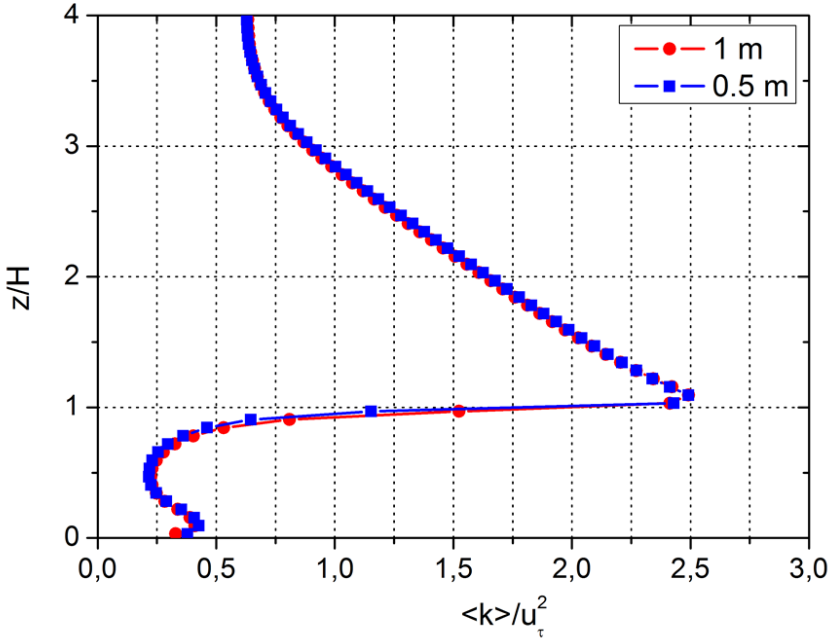

Figure 1. Vertical profiles of the spatial average of $^{k}/_{u_\tau{}^2}$ using 0.5 m and 1 m of grid resolution in the 2D geometry.

Fig. 1.

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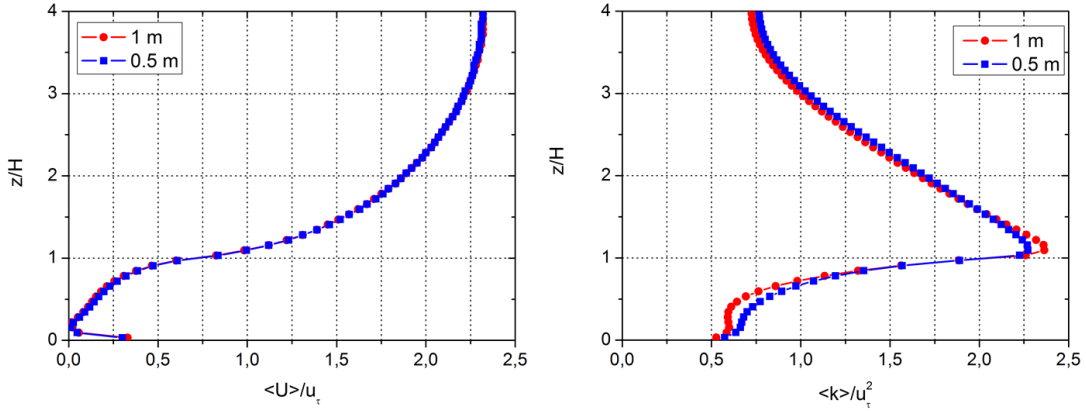

Figure 2. Vertical profiles of the spatial average of $^{U}/_{u_\tau}$ (left) and $^{k}/_{u_\tau{}^2}$ (right) using the fine and the coarse grid.

Fig. 2.

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