Atmos. Chem. Phys. Discuss.,
doi:10.5194/acp-2016-202-AC1, 2016

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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Received and published: 2 September 2016

Thank you for your assessment about the manuscript and your comments. The manuscript has been modified to create a better overview of all cases considered in this work and so, providing some quantitative conclusions from the results. All typing remarks have been modified in the revised manuscript.

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:

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Discussion paper

Abstract. *Line 16-17: rephrase*

Please see this section in the PDF file.

Introduction. *Line 33: 'marked'? Not clear what you mean. Line 35: 'O3 sensitivity', do you mean the sensitivity of O3 to ??? or the sensitivity of the results to O3? This is not clear.*

It is referred as the sensitivity of O3 to the NOx emission level, since they evaluated the changes in O3 concentration on varying the NOx and VOC emission levels. It has been clarified in the revised manuscript, please see PDF file (Page 2, lines 24-27).

Model Description (Section 3.1). *Page 5, line 25-end: rephrase*

Please see the PDF file (Page 5, lines 18-22).

Simulation Setup (Section 3.2) *restructure this section.*

This section has been re-organized as per your remarks. Please see this section in the PDF file.

Page 6, line 17: Are the symmetric conditions also applied to the concentrations?

For pollutants concentration, the symmetric conditions are only imposed in y-direction. The outlet condition was established at the top of the domain and a constant value of concentration was imposed for each pollutant. Please see the PDF file (Page 6, lines 23-25).

Line 4-5: The NO/NO2 concentrations also depend on the intensity of turbulent mixing in the boundary layer, e.g. the difference between clear and cloudy days, or strong/weak inversion. How has this been addressed?

We agree on this with the reviewer. However, the influence of the turbulent mixing intensity at the boundary layer on NO/NO2 concentration is not addressed in this paper. The same type of turbulent mixing (induced only by the interaction between the wind and the presence of buildings without any thermal effect) at a peak hour of traffic emissions is considered in all scenarios.

CFD Model Evaluation: *(Page 7, line 21):'from a well-established chemical box model': describe which one in some words. After reviewing the paper I do not have a clear idea on where the results of this box model are used. Is this an essential part of the paper?*

This section is important in this paper since it evaluates the implementation of the chemical terms in the CFD model. To achieve this, the CFD is run as box model (e. g. without transport and diffusion) and the results of pollutants concentrations were compared with the outcomes derived with the chemical box model used to test the chemical mechanism.

This issue has been clarified. Please see the PDF file (Page 8, lines 8-18).

Results. *Page 9, line 13: I found the use of the word 'canopy' confusing. E.g. in page 10, line 11 you write 'below the canopy'. This suggests that you simulate concentrations below trees. Is this true? Please clarify. How tall is the canopy?*

What is meant in the text, in reality is below canopy top, or within the canopy. In this work, the height of the canopy is regarded as that of buildings (H). This concept has been clarified in the revised manuscript (Please see the PDF file, page 9, lines 3-4).

Page 9, line 19: Is the source emission rate Q expressed per unit area?

Q is the emission source rate and it is expressed in kg s-1, so that Q/Aem is the emission density flux, in Kg/s/m2. We have noticed that there was a mistake in the expression for the normalized concentration. The normalized concentration is now:

$$C_N = \frac{C\ u_\tau\ A_{Em}}{Q} \tag{1}$$

Please see the PDF file (Equation 8; Page 9, line 12).

Could you explain why in the low O3 case the VOC emissions do not make much difference?

In the low O3 case, the selected zenith angle is representative of winter conditions, therefore the photolysis constants are smaller than that given in a representative summer case. This implies that the background O3 concentration computed by the photochemical equilibrium equation is low. In turn, the VOC oxidation cycle is also limited by the photolysis of some VOCs. Besides, given that the NOx emissions dominate over the VOC emissions, the high levels of NOx concentration tend to inhibit O3 formation and limit the O3 production through VOC reactions. Therefore, the difference in NO and NO2 concentration after including VOC reactions against the photostationary steady state is negligible in this low O3 case. So the weak dependence on VOC concentration is a combination of the low O3 and small photolysis rates.

We have included this text in the revised manuscript. Please see the PDF file (Page 10, lines 16-23)

Page 11, line 11 to end: this is discussion, not results. I would expect that you describe the difference between the 2D and 3D experiments here.

This section has been modified in order to show more results. Please see the PDF file (Page 10-11).

In this work, the differences between 2D and 3D geometries were not addressed since it would be a complex study in order to carry it out here as well. In this section, the influence of several wind speed on NO and NO2 dispersion in the streets is studied in different types of geometries. The objective is to understand whether the deviation on normalized concentrations from that of the tracer by including chemical reactions had the same behavior or not in both geometries. Note that the concentration of a non-reactive pollutant is inversely proportional to wind speed (Parra et al., 2010), but the chemical reactions modified this behaviour. Finally, the same conclusions, in terms of chemical effects, were obtained from the CFD results for both geometries.

Page 14: Line 2-4: rephrase.

Please see the PDF file (Page 13, lines 22-23).

Page 15. Line 4-5: rephrase.

Please see the PDF file (Page 14, lines 22-23).

Page 15. Line 8-20: Can you make this part more quantitative, and include recommendations to direct further research?

This part has been modified in order to provide more quantitative information from the experiments performed in this work. Please see the PDF file (Page 14, line 30 to end)

The subject of computation time is not addressed here. Perhaps implicitly, but not explicitly.

We agree with the referee's comment, since we have not evaluated explicitly the differences in computational load on using one chemical scheme or other one. But it is implicitly included in our conclusions, because the aim of this work is to optimize the modeling of NO and NO2 dispersion and so as to reduce the computational time required to carried it out.

We have indicated the relationship between computational time needed to simulate the complex chemical scheme and the photostationary steady state (Page 3, lines 17-19)

Figure 6: subplot e should be the same as 4e? They refer to the same experiment if I understand it correctly.

The figures for the same simulations are Figure 6 (e-g) and Figure 4 (b-d) corresponding to the case of O3=39.9 ppb with u_τ=0.23 m s^{-1} (Case 2).

Please also note the supplement to this comment:
http://www.atmos-chem-phys-discuss.net/acp-2016-202/acp-2016-202-AC1-supplement.pdf

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