

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

Anonymous Referee #2

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GENERAL COMMENTS The paper entitled "CFD Modeling of Reactive Pollutants Dispersion in Simplified Urban Configurations with Different Chemical Mechanisms" deals with the modeling of reactive pollutants using a computational fluid dynamics (CFD) model. Three chemical approaches are considered. Main results show that the presence of ozone in the street acquires an important role in NO and NO₂ dispersion.

The paper is an application of a CFD model to the study of dispersion of reactive pollutants in idealized geometries. Chemical schemes are implemented in the CFD model and this is an important and novel contribution since most studies focused on non-reactive pollutants. Overall the authors have done a lot of technical and scientific work, but in my opinion it is presented in a slightly confused way. It is not obviously

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clear which cases have been studied and main results obtained. The description of the cases is not done in a schematic way and this makes the paper, at least in the methodology sections, hard to understand. Also some sentences are not scientifically sound. More attention should be paid to what is discussed and introduced based on previous literature studies and references should be given. Also English should be checked. I suggested several corrections, but I cannot guarantee everything has been checked so I suggest the paper to be checked by a native speaker. Further, there is no attempt to analyse physical processes behind the results. The above and below issues should be addressed by the authors before publication. The authors have the necessary expertise to address all the issues which concern mainly the presentation and analysis of results and not the methodology employed which is of high scientific level.

SPECIFIC COMMENTS Abstract. - Overall I found the abstract a little bit confused. Several information are 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. - The sentence "it is reduced to 23 species ..." Is not clear since the reader at this stage of the paper may not know the starting point from which the reduction takes place. - "the concentration of reactive pollutants is affected by many atmospheric parameters" is too generic. Which parameters? And which are you considering here? - "role in NO and NO₂ concentration" and not dispersion - "The joint evaluation of both parameters": what is "both" referred to?

Introduction. - Please check throughout the paper that NO_x, NO₂ etc. have been defined before using chemical formula. - define UCL - Pag. 2 Line 28. This is a repetition of what already mentioned at line 24 - Pag. 3 Lines 17-18. This concept is a repetition of what already mentioned at line 5 of pag. 2. Overall also the introduction is slightly confused. The same concepts are repeated throughout the section. - Pag. 3 Line 19. How did you estimate "a factor of 2"? - At the end please underline the structure and the original contribution of the paper

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Chemical Schemes used. - RACM? - Reduced to 25 reactions with respect to...? Please introduce the scheme otherwise it is not easy to understand - Overall also this section is hard to follow. As in the abstract the cases investigated are mixed, while they should be presented in a more schematic way avoiding to first introduce, then discuss of a scheme, then move to the other and coming back to the first and so on... - It is not clear why two so close wind velocity 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. - How did you estimate 930 vehicles?

CFD model evaluation. Please remove the sentence "despite the fact that ... was previously validated..." This is not scientifically sound. The present paper is based on CFD simulations and thus the simulations should be critically validated. For this reason, I suggest also to validate flow and turbulence obtained from CFD and not only concentration at few points. This would add value to the paper and justify the accuracy of results. - Did the authors performed any sensitivity test of the grid and domain size? - Remarks should be added about other turbulence modelling, such as the RSM, LES

Results. - Please 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. - Pag. 9 Lines 14-15. What do you mean with "apparently"? 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 he 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? - Pag. 11 Line 6. 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. - Pag. 11 Line 28. "The effect of

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considering reactive pollutants is enlarged.." You mean the importance of considering reactive pollutants for a better model accuracy...? Please check this kind of sentences throughout the paper.

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