Atmospheric Chemistry and Physics Discussions

Atmos. Chem. Phys. Discuss., referee comment RC2
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Comment on acp-2022-365

Anonymous Referee #2

Referee comment on "Modeling of street-scale pollutant dispersion by coupled simulation of chemical reaction, aerosol dynamics, and CFD" by Chao Lin et al., Atmos. Chem. Phys. Discuss., https://doi.org/10.5194/acp-2022-365-RC2, 2022

The authors coupled the SSH-Aerosol modular box model into Code_Saturne and OpenFOAM CFD models. This coupling allows the representation of primary and secondary pollutants such as NO2 and secondary aerosols (including size distribution) inside an urban canyon in Paris. Results of twelve-hour simulations of NO2 and PM10 between OpenFOAM and Code_Saturne with SSH-Aerosol were similar and closer to measurements. Configuration experiments and case studies were focused on OpenFOAM coupling (CFD_Chemistry). CFD-Chemistry was evaluated in grid size, time step, and coupling method. Averaged concentration fields of gasses and particles and the size distribution of PM10 were evaluated. Finally, a case increasing NH3 traffic emission was presented as an example of using the model for regulatory purposes.

The manuscript is well written and organized, the tables and figures support the results and the results and conclusions represent an improvement in the field.

Minor comments and required clarifications are detailed below:

Specific comments

- Line 143. Please clarify the reason for not including nucleation in simulations.

- LIne 146 - 153. Recommend adding a schematic diagram to clarify the coupling detailed in this paragraph, like Fig 3 in Kim et al (2018).

- Fig 3. could also include NO2 and O3 background concentrations that would complement the discussion of Fig. 12. It could also help to have the gasses emission rates like NOX as it was also used to estimate NH3 emissions.

- Line 177. Please specify the spatial resolution of WRF simulations.

- Line 193 Please specify the model name to produce the background concentrations.

- Line 241-243 Fig. 4.b showed that the PM10 CFD-chemistry did improve PM10 simulation but only during the morning hours, CFD-chemistry is closed to CFD-passive during the afternoon. When compared with Fig 3 a. It seems that it follows the behavior of background concentration, even when there is an increase of PM10 emitted compounds during the late hour of the afternoon (Fig 3 b). Did the authors perform sensitive tests of background concentration?

- Line 293: Please elaborate on the reasons for choosing OpenFOAM instead of Code_Saturne. Maybe it is easier and faster to run or it performs better than Code_Saturne (Table 1 only showed performance statistics for OpenFOAM). In that sense, It is also important to show the difference in computational time of running CFD-Chemistry and CFD-Passive.

- Line 591 - 592. The authors said that background concentration came from measurements, nevertheless in line 193 they said that they were obtained from the regional-scale simulations, please clarify.

Technical corrections

- Line 124 and Line 127. Please include the definition of RNG (Re-Normalisation Group), PISO (Pressure Implicit with Splitting of Operator), and SIMPLE (Semi-Implicit Method for Pressure-Linked Equations) acronyms.

- Recommend to add units in colorbars in Fig. 12 and 13, like in Fig. 11.

- Line 466, It should be: the HNO3 concentration peak in CFD-chemistry was later than that in CFD-PASSIVE.

- Line 458 Said NH3 concentration peaked around 6 am, later in line 466 is said to be at 7 am.

- Line 505, and line 508 PM10 are repeated, maybe it is OM.

- Line 834, von Karman constant should be von Kármán constant

- Equations for dry deposition schemes for gasses in Appendix A should be labeled as A5 and A6.