Geosci. Model Dev. Discuss.,
https://doi.org/10.5194/gmd-2020-387-RC2, 2021

Geoscientific Model Development Discussions

Interactive comment on "APFoam-1.0: integrated CFD simulation of O_3–NO_x–VOCs chemistry and pollutant dispersion in typical street canyon" *by* Luolin Wu et al.

Anonymous Referee #2

Received and published: 5 January 2021

General comments:

Wu et al. present the development of an open-source CFD code based on OpenFOAM for Atmospheric Photolysis calculation to study the dispersion of reactive pollutants at the microscale. Full O3-NOx-VOCs chemistry has been implemented in the CFD model and compared with data from a box model simulation. Additionally, the accuracy of the model to predict the flow field and pollutant dispersion is evaluated in a 2D street canyon against wind tunnel measurements. This coupled system is applied to perform a comprehensive sensitivity test and examine the influence of the background precursors of O3, traffic emissions, and wind speed on pollutant concentrations in the

street.

I think this work provides valuable information on the field of urban air quality modeling at the microscale and I suggest carefully addressing the following comments before publication in GMD.

1.Although distinct photochemical mechanisms have been implemented in the model, this paper just present results from the full chemical mechanism "CS07A". Has the implementation of the rest of the photochemical schemes been properly evaluated? It should be mentioned in the manuscript, at least.

2.One of the limitations is that despite the model is fully coupled, the evaluation is performed separately (chemistry, flow, and dispersion of pollutants). It is probably because of the lack of measurements to validate this system; however, it should also be mentioned in the manuscript.

3. Conclusions. I would recommend improving this section and being more precise in giving the outcomes.

Specific comments: #Line 9. How can this development improve the resolution? #Line 13. The implementation of the atmospheric photochemical mechanism in the CFD model is evaluated with box model results. It should also be mentioned in the abstract. #Line 130. Similar to the reaction rates depending on T, might the photolysis rates be modified according to an input of the intensity of the light? #Line 151-156. It should be mentioned (here or in Section 3.1.) whether the implementation of these three photochemical mechanisms has been evaluated. #Line 213. Why is the simulation time set at 24h if no diurnal variation is considered? #Line 215. "Figure 2 shows the concentrations of 52 species. . ." Is that average concentration over 24h or concentration at a specific time? #Line 229. The concentrations are extremely low (10ˆ-40 ppmV). I would recommend focusing on the comparison of CFD outputs and box model results just under realistic conditions since the largest differences occur when concentrations are almost zero and are mainly related to the different processing of these two mod-

els. #Line 254. “. . ., the prediction accuracy is better in simulating the low-wind-speed region”. Please add a reference. #Line 296. The model acceptance criteria were previously defined in Chang and Hanna (2004) and Hanna and Chang (2012). Chang, J., Hanna, S., 2004. Air quality model performance evaluation. Meteorology and Atmospheric Physics 87 (1), 167-196. Hanna, S., Chang, J., 2012. Acceptance criteria for urban dispersion model evaluation. Meteorology and Atmospheric Physics 116 (3-4), 133-146. #Line 298. “. . .the respective NMSE, FB and R are 0.06, -0.13 and 0.95 (Table 1). . .”. These values do not correspond to the values presented in Table 1. #Line 302. Is any photochemical mechanism used in this simulation? If not, it should be clarified that this evaluation is performed with no chemical reactions included. #Line 325. Please use the same nomenclature for the aspect ratio (H/W). It is also referred to as H/W=1 in the abstract. #Line 331. Since the pollutant concentrations are presented in ppbv, could you also provide the emissions of NOx, VOCs and CO in ppbv s-1? #Line 351. Could you explain why that time step is selected for the chemistry? #Line 368. Please also provide the percentage of VOC reduction over the total VOC emissions (as shown in Table 3). #Line 385. I do not agree with the sentence “While on the windward side, NOx concentrations are more affected by the background conditions rather than emissions”. NOx concentration on the windward side is more affected by the background conditions than that on the leeward side. However, the influence of the NOx emission on NOx concentration on the windward side is still larger than the background concentrations. Based on the results in Section 4.3., the influence of background concentrations on NOx concentration on the windward side is just around 10-20%. #Line 396. “...NO could be up to 90%” higher in the simple chemistry case. #Line 409-412. “. . .from the oxidation of background VOCs with OH will consume”. Why is that oxidation only occur with background VOCs? Not sure how to distinguish the background VOCs from the emitted VOCs on the concentration in the street since pollutants are already well mixed and chemical reactions are non-linear. #Line 420-423. I think it occurs in the Base case as well. #Line 446. “In summary. . .”. Please explain this better. #Line 468. Is average or total concentration in the street? Please

modify the caption in Fig. 15 as well. #Line 490. This paper presents results from the coupling of the chemical mechanism CS07A and CFD model. It should also be clarified in this section. #Line 494. “. . ., 2D and 3D pollutant dispersion. . .”. The simulations are only performed in a 2D street canyon. #Line 497. Add aspect ratio. #Line 498. Please provide the VOC-to-NOx emission ratio used in these simulations. #Line 499. “Other numerical sensitivity cases,. . .”. Please clarify what cases. #Line 503. Due to the non-linearity of chemical reactions, how is the contribution from the boundary conditions to O3 concentration computed? #Line 504. “Ventilation condition is another reason for the NOx concentrations increment, and the increase of NOx can be up to 98%”. I think that is to be expected. In steady state (or quasi-steady state) conditions, the concentration of a non-reactive pollutant is double when wind speed is divided by 2 (if emissions do not change). Despite NOx is not truly a non-reactive pollutant, due to the influence of the VOC reactions with NO and NO2, it might be almost considered as non-reactive as the sum of NO and NO2.

Technical comments:

#Line 44. “material” instead of “materiel” #Line 297. Change “pervious” to “previous”. #Line 371. Add “...change rate (CR_p). . .” #Line 485. “polies” to “policies” #Line 392. Change “Figure 11 shows the changes rates of pollutant concentrations and NO to NO2 ratio. . .”

Table 3. Add the name of the “full chemical mechanism” used in the simulations and mentioned in the manuscript (CS07A photochemical mechanism). Figure 11-14. Please use the defined CRp (Eq. 28) to show the change rate of each pollutant in %.

Interactive comment on Geosci. Model Dev. Discuss., https://doi.org/10.5194/gmd-2020-387, 2020.