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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.

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1 General comments

This paper developed a calculation framework (APFoam-1.0), based on open-source CFD code OpenFOAM, for atmospheric photolysis to examine the micro-scale reactive pollutant formation and dispersion in the urban area. Five new types of reaction are added to the chemistry module, which is coupled with full O3–NOx–VOCs chemistry and CFD model. The model was validated against SAPRC box modeling software and wind tunnel experimental data. The framework was applied to case studies investigating O3–NOx–VOCs formation processes and dispersion of the reactive pollutants in an example of a typical street canyon. APFoam provides a numerical simulation tool

based on the general purpose open source solver, which gives researchers the full capability to have control not only out of the box but also inside of the "box". So APFoam can be a useful tool of broad interest in atmosphere science.

However, the merits of APreactingFoam and APSteadyReactingFoam modules (two important modules of the APFoam-1.0) are not well demonstrated/articulated. Fully coupling (two way coupling) is adopted in both APreactingFoam and APSteadyReactingFoam, where the reaction heat is considered to have impact on fluid flow. Intuitively speaking, the concentration of pollutants is too low to have a significant impact on the fluid field.Whether the heat source from reaction is considered or not might NOT have any significant effect in terms of simulation accuracy: whether to consider or ignore such tiny effects won't change the simulation results too much. But it will have a significant effect on computational cost affecting the speed of simulations. Two way fully coupled model requires solving coupled governing equations with more unknown variables, which usually requires much more computational resources. In addition, the fully coupled system has more constraints on time steps and hence needs smaller time steps. The numerical algorithms become more complicated, too. As a general tool (calculation framework) for doing simulation, computational efficiency is important. Complicated model also makes results analysis more complicated as there are more factors that need to be considered.In that sense, the simplest 3D module, APonlyChemReactingFoam, might be the best choice for most situations due to the following reasons:

- Faster in term of simulation and reduce computational cost significantly as explained above.
- Flow field data can be calculated offline and reused if the CFD set up does not change. For example, in certain case study, you keep the geometry, boundary condition and initial condition unchanged and only vary the source of pollutant (such as the locations, the pollutant release rate et al), then you only need to

do the CFD simulation for once and reuse it for different case studies, this will significantly speed up your case study.

Validation of the calculation framework is validated only using APonlyChemReactingFoam. APreactingFoam and APSteadyReactingFoam are not validated in the validation section. Not clear if APreactingFoam and APSteadyReactingFoam have ever been used in the case study section or not, the author did not explicitly mention that. Do these two modules (with much more complicated governing equations) really have certain advantages in any situation? If so, I would encourage the author to justify it in a proper way, either based on literature review or ideally with a real case study. The authors need to show that considering and not considering the heat effect from reaction will have significant effect on simulation results for certain cases. With the above being said, It would also be necessary to compare the simulation speed of those three modules. In addition, in the validation section (section 3), the only validated 3D module APonlyChemReactingFoam is not validated in a fully coupled manner. The reaction model is validated alone (section 3.1). The CFD model is validated alone (section 3.2), too. And the pollutant species transportation and dispersion validation (section 3.3) is , at least, decoupled from reaction. The model is fully coupled, but the validation is done in a decoupled manner. Maybe the coupling between reaction and pollutants is also very weak and can be decoupled as well?

In summary, the models seem more complicated than necessary and lack sufficient validation. I would recommend accepting this manuscript to publish on GMD only after the major concern and specific comments (see next section) being properly addressed.

2 Specificl comments

Abstract, line 9. Numerical "resolution", in the context of mesh-based methods, such as the finite volume method used in the paper, depends on grid size, which is purely a choice in preprocess. Not clear to me how the framework developed in this paper can "improve the resolution". By "resolution", do you mean to say that the framework you developed targets at modeling small scale phenomena (such as street scale flow)?

Abstract, line 14. The framework is also validated against SAPRC box modeling software, which is an essential validation, why only mention the wind tunnel validation in the abstract? Worthwhile to mention both validations.

Abstract, general comments. Please double check the grammar in the abstract.

Section 1, general comments. It would be helpful for readers to have a better understanding on the major contribution of this paper if you have a little bit more detailed discussion regarding existing CFD based simulation studies in this area. For example, do they consider atmospheric photochemical in their simulation? Are those five reactions recently added in this paper already been studied in other research? In the existing studies, do they consider two way coupling or one way coupling? What tool do they use in their simulation study, OpnFoam or commercial softwares?

Section 2, question. How do you determine the time step for this coupled system?

Section 2.1, line 113. Missing“ boundary condition", which is included in Fig. 1 but not mentioned in this paragraph.
T in Eq.1 is supposed to be the temperature of the mixture? In Kelvin or Celsius?

In Eq. 2, Question. How are the lower and upper limit of the integration determined?

Eq. 1 - Eq. 5 use k to represent “reaction rates", while in Eq. 6, w is used as the reaction rate. Are those two reaction rates the same thing? If so, why using different symbols?

In Eq. 8, should the average of molecular weight also be an unknown variable that needs to be calculated based on the mass fraction of each species? Imaging that chemical reaction changes the mass fraction of different species and then leads to changes of the average molecular weight. Any justification why the average molecular weight is assumed to be constant. Actually the assumption that average molecular weight is constant sounds reasonable to me, as the average molecular weight change caused by reaction might be ignorable. Then the following up question is, how significant is the reaction heat source? Seems can be ignorable as well. Authors may need to prove whether they are significant or not.

Section 2.3. For the governing equations (Eq. 6 - Eq. 8) of APChemForm, there are in total n+2 governing equations, I suppose the primitive unknowns in the governing equation are: T, ρ, p, h, Y_i, there are in total n + 4 unknowns. number of equations < number of unknowns, Seems some other equations missing or not mentioned? Mathematically, the system is not closed. Or the author assumes that two of those T, ρ, p, h are not unknown? Which two?

Section 2, general comments.

- Symbols that are used in this paper only need to be specified for once, for example, ρ is density, you only need to explain it the first time it appears.
- Need to make sure that the same symbol has consistent meaning across the manuscript, make sure the same variable is only represented by one symbol.
- There are several dummy assumptions made in the model: such as, the mixture (mixture of air and pollutants, air itself is mixture) is in a thermal dynamic and dynamic quasi static state, they all share the same temperature and velocity. Maybe worthwhile to explicitly state the assumptions that you made when you establish the model.
- Would be better to explicitly specify that, ρ is density of the **mixture**. Similar for **U** and T.

Eq. 10 and Eq. 20, the physical viscosity is also considered. For air, physical viscosity is much smaller than turbulent viscosity and usually ignored in air flow simulation.

Eq. 20, k shows up again here, what does k represent in this equation, recall that k was used as reaction rate in section 2. This is really confusing.

Section 3.2. May worthwhile to explicitly state that the Eq. 18 - Eq. 21 are not a new set of governing equations, they are essentially governing equations Eq. 13 - Eq. 15 with turbulence model.

Section 3.2, line 256. Do you treat the air as incompressible flow in the simulation?

Section 3. In the validation case, what is the Renolds number for the CFD simulation set up? It is not clear to me why you choose to scale the geometry in CFD simulation?

Why not use the same geometry as whatever in the experiment?

Section 3. Why no 3D simulation attempted? Any difficulties or due to computational cost?

Section 3. The validation mainly validates the pollutant transportation and dispersion in the fluids field coupled with reaction, no reaction-flow-transportation coupling situation be tested. Namely, APSteadyReactingFoam, APreactingFoam are not tested. So do the authors also believe that the effect of reaction to flow is too weak that no need to be overly concerned about it?

Section 3.3, general question. Could you clarify which of the following strategies is used in your validation?

- Solve the turbulent fluids governing equation (Eq. 18 - Eq. 21), pollutant species transportation equation (Eq. 12) and reactions (Eq.1 - Eq. 5) simultaneously.
- First do the fluids field simulation without considering pollutant species and reaction, that is, first solve Eq. 18 - Eq. 21. Then do species transportation and dispersion together with reactions based on fluids field solution obtained in the first step? Namely, solve Eq. 12 and Eq. 1 - Eq. 5 in second step.

Section 3.3, general comments. What is the time scale for reactions and what is the time scale for species transportation and dispersion? The motivation to ask this question is to see if there is possibility to decouple reaction from species transportation in such micro-scale simulation. In this section, both the experiment and the numerical simulation do not consider chemical reaction. Does this indicate that the coupling between reaction and species transportation and dispersion is ignorable as well? That

is to say E_i in Eq. 12 can be removed.

Section 3, general comments. Comparison between those three modules: APSteadyReactingFoam, APreactingFoam and APonlyChemReactingFoam would be very helpful.

Section 4, general comments/questions. Could you explicitly specify which one of the three (APonlyChemReactingFoam, APSteadyReactingFoam and APreactingFoam) is used in case studies. Any discussions to compare APonlyChemReactingFoam with APSteadyReactingFoam/APreactingFoam.

General comments regarding the associated source code. “README" has detailed instructions for compilation, but does not specify any dependencies, such as third party libraries that needed? Any requirement in terms of the version of these dependencies? In addition, I would recommend adding detailed instructions about how to run APFoam, either in “README" or in a separate user manual. Imagining I am a fresh user of APFoam, I would need to know which executable to execute. Before executing that executable, what kind of preparation work is needed. For example, no need to instruct users how to generate mesh, but would be necessary to mention that users would need to get the meshed geometry ready before using APFoam. A little bit more Instructions about how to make use the “APFoam_tutorials" would also be very helpful.

3 Technical corrections

Abstract, line 9. Change “newly" to “new".

Abstract, line 13. Change “reaction" to “reactions".

In Eq. 1, please specify the meaning of T?

In Eq. 7, what is the h? Specific enthalpy?

Fig. 9, caption. “The probe points **locations**.“

Line 307. “... in **the** targeted street canyon ."

Line 334. Change “obtain" to “obtained".

Line 414. “... **is** slightly greater than that of ..."

Line 418. Again “... **the** street canyon .."

Line 419. "This is because **that** the background "