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Interactive
comment

Interactive comment on "The Framework for 0-D Atmospheric Modeling (F0AM) v3.1" *by* G. M. Wolfe et al.

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This work presents a box model environment for the testing of chemical mechanisms. F0AM represents an advancement over some of the other available mechanism testing codes in that the user has the ability to change the photolysis calculation method amongst other things. The paper takes the reader through a number of model examples which I can see would be adaptable to most experimental set-ups: a fixed location (Eulerian) setup, and a Lagrangian set-up, where the box is able to move in 3D space. Data from several field campaigns are used to demonstrate how F0AM operates in both set-ups.

The paper is a well written, enjoyable read and I recommend publication in GMD after consideration of the following points:

I found figure 2 and its associated write-up in paragraph 3 of page 4 confusing. Where it says "differences between the TUV and hybrid values for C2H5CHO and CH3COCH3....." I can't see an entry for C2H5CHO in the x axis of figure 2, but I can see two separate entries for CH3COCH3 (one next to HPALD in the upper plot, the other next to CH3CHO->CH3CO in the lower plot; only the first of these entries shows both TUV and MCM together). There are no plotted TUV values for the first 3 species listed on the lower plot (crotonaldehyde, benzaldehyde and diethylketone), and it is not clear why they have been included.

Page 5, line 17, would it be possible to include mechanisms in a kpp format in a future release?

Page 7, photochemical chamber paragraph. I've done a few chemical box model studies on photochemical chamber experiments and have found that you need some way of accounting for the initial wall loss of species when they're first injected into the chamber. Is this accounted for in the model, or does the user need to make an assumption that the injected concentration does not equal the initial concentration of reactant?

Figure 6. This is where it gets really interesting, from a mechanism point of view. The first thing to note is that you've chosen two versions of the MCM and two versions of the carbon bond mechanism, and both show an increase in OH concentrations with the evolution of the newer versions.

The second point is a request for some additional observations to be plotted. Figure 6 shows a time series representing the SENEX campaign. I'm not sure whether radical species where measured, but plotting some of the secondary species (isoprene products, formaldehyde?) would show how well the chemistry schemes are performing. This is a common criticism of mechanism comparison papers – the mechanisms are compared with each other but not to observations which would tell us which scheme performed 'better' for that particular model set-up. After all, this is what users are really after!

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Discussion paper

There are a couple of problems in the reference list where subscripting hasn't worked properly: see page 12 line 11 and also line 49.

I also wanted to have a go with the F0AM software, as its capabilities are of interest to me. I downloaded version 3.1 from the supplementary section. I used Matlab many years ago during my PhD, however I didn't find this code intuitive. What I was after was details of how to execute an example script. There are example scripts with the download, but the suggested technique in the readme.pdf is to "dive in", which is a bit daunting. It would be useful if this readme document started with a guide about how to set up the framework (windows/linux?) and run an example, as my initial thought was that it was going to take me a while to set-up properly.

I tried executing the "exampleSetup_chamber.m on linux and got the message there was an undefined function of variable F0AM_ModelCore. It took me a little while to work out that I needed to add every folder to the model pathname in order to run the script. Once I did this, I was able to run the model and out popped four figures. I had problems with a couple of the other example scripts, mainly due to licensing problems at my end I think (maximum number of statistical tool licences had been used, so the diurnal cycle script and the mechanism intercomparison script crashed). If this isn't the case then I'm happy to be contacted by the authors to get it working.

The script was very well commented, with instructions on how to change the input variables.

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