Interactive comment on “ASIS v1.0: an adaptative solver for the simulation of atmospheric chemistry” by Daniel Cariolle et al.

Anonymous Referee #3

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This paper describes the implementation of the "Adaptive Semi-Implicit Scheme" (ASIS), a chemical solver for use in atmospheric simulations. The paper has a general discussion on the requirements on a chemical solver, before describing the ASIS formulation, and then giving some examples of its implementation in box models and GCMs.

I found the discussion informative, and the authors reasoning behind the formulation is well explained, along with the benefits that ASIS brings over other schemes. I would recommend this paper for publication, with some modifications.

General Comments

Due to the large number of tests performed it was a little difficult to keep track of the settings used in each case. I would recommend giving a master table (or tables) giving...
the configuration for each shorthand used in the plots (e.g. R1, G1, A1, A2, A3, A4, MR, MA, EB, ASIS etc.) and what the settings are used for each (e.g. values for ATOL, RTOL, using ode23s, ode15s, DGESV, GS, GMRES etc.), the experiment run (e.g. FLUX, STRATO, MOCAGE, Mars Box Model, LMD Mars GCM etc.), and also the chemistry scheme used (e.g. RACMOBUS, Mars). This would be especially helpful for comparing between sections, as it can be difficult to pick out this mass of information from the text.

I would also like more discussion of computational cost - the timestep is discussed in detail, but is rarely then compared to the overall run-time. It is certainly interesting to see where the timestep changes, but in terms of usability it would be handy to know exactly how much more time it took. This could be included in e.g. table 4 for the section 3 cases, perhaps as a ratio relative to the R1 case. These numbers should also be clearly stated for all other cases.

The run length is also a bit short for most cases. The 1 day simulations for the box model are very short, especially when it appears that the A2 case is diverging from the R1/G1/A1 cases. Have these simulations been run for longer, and if so, how do the results of A2 (& A3) evolve? Also, A3 is not plotted at all, but these settings are then used for the MOCAGE simulations. The A3 results should also be included in the plots in Figures 1 & 2 (or plotted separately with a larger scale if required).

The GCM lengths are slightly better (3 months and 150 days), but still short. Are there plans to do longer runs with a full evaluation and budget analysis? The results presented here have highlighted deficiencies in the existing models, but a full analysis on longer simulations would be required to properly validate ASIS, as opposed to this paper which describes its implementation.

I do especially like that the authors have tested ASIS in a number of different models, both box models and global models, with different chemistry schemes and also for different planets.
Specific Comments

• page 1 line 16: "now include"

• page 1 line 16: "several hundred reactions"

• page 2 line 30: I'm confused by "It is also desirable to let the user a minimum of free parameters to tune". Do you mean "desirable to give the user"?

• page 4 line 18: I think you mean "Sandu and Sander (2006)", although I can't find this reference in the reference list. I assume it is Sandu, A. and Sander, R.: Technical note: Simulating chemical systems in Fortran90 and Matlab with the Kinetic PreProcessor KPP-2.1, Atmos. Chem. Phys., 6, 187-195, doi:10.5194/acp-6-187-2006, 2006. I haven't gone through and double-checked all the other references, but I suggest that the authors do so.

• page 8 line 9: Could the authors make it clear here that when saying "To validate and evaluate the performances of ASIS and the associated numerical codes several case studies have been used. All these cases are based on the RACMOBUS chemical scheme used within the MOCAGE CTM" the authors refer to section 3 (& 4) only, as a different model and scheme are used for section 5.

• page 14 Figure 3: The quality of this figure is not very good, and also the final "s" in species is truncated on both figures.

• page 15 Figure 4: "Number of timesteps"

• page 19 line 3: I think you mean "Figure 8" here.

• page 20 Figure 8: There is a bit of an issue in terms of the figure quality, some of the bottoms of the numbers of the colour-bars are cut off at the bottom.
• page 20 line 6: "a fixed timestep"

• page 22 line 1: Do you mean "4.7 times"? Is this a mean over the whole 3-month run?

• page 26 Figure 11: When is this from - is it a snapshot from the start/middle/end of the 150-day run?

• page 27 Figure 12: Similarly for Figure 11 - when is this from with respect to the start of the run. Is it the same as for Figure 11?

• page 28 line 3: Currently the sentence implies that ASIS has been implemented in two 3D models of the Earth and two 3D models of Mars, rather than one 3D model for each.

Interactive comment on Geosci. Model Dev. Discuss., doi:10.5194/gmd-2016-281, 2016.