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

Anonymous Referee #1

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General comments and recommendation.

The authors of this paper describe a newly developed chemistry solver. While reading the paper I became convinced that the ASIS solver is working well. The trick with the Delta factor, eq. 9, is an interesting way to cope with the large range of lifetimes of the tracers in an automatic way. ASIS is very flexible and does not need explicit equilibrium solutions of fast reactions. I can agree with the authors that the high accuracy of solvers like Rosenbrock is often not needed for CTM simulations. The examples (box model, MOCAGE, Mars model) are very instructive and clearly show the properties of ASIS. As such I am in favour of publishing this work in GMD.

However, there are a few major comments and a couple of more minor points which I would suggest the authors address before the paper is published.

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Discussion paper

First, from the paper it is not so clear why a new solver is needed. In fact, in the paper there are comments which may make the CTM modeller decide to stick to solvers like Rosenbrock. In particular I would like to see a more detailed comparison against Rosenbrock concerning run time and accuracy, for small and large numbers of chemical species. What are the main reasons to replace Rosenbrock by ASIS? The abstract could be extended also in this direction.

Some comments on the advantage of ASIS I found a bit misleading, e.g. on p15: “At the moderate accuracy required for atmospheric simulations the ASIS solver compares well with higher order schemes, and limits the computational cost while assuring mass conservation”, but this improved run time is linked to lower accuracy. For the same accuracy I got the impression that run times were comparable.

I would expect to see more references (especially about chemical solvers and their properties) in the introduction.

More specialised comments:

- Title: “adaptative” -> “adaptive”

- Abstract: From the abstract it is not clear what the advantages of ASIS are with respect to the Rosenbrock and Gear solvers. Why do we need an other solver?

- Introduction: There are no references given in the introduction to the general literature on chemical or differential equation solvers. An introduction should sketch the starting point of the work - the state-of-the-art - and in this way clarify how the new developments described in the paper advance this present knowledge and models. I suggest that the authors add a section with references discussing the current status concerning solvers in relation to chemistry models. Several references are provided later on in the paper, but the current list is not very extended and could be expanded somewhat.

- p2, l3: “ODE” is not defined

- At several places: I suggest to replace “resolution” by “solution”

- p2, l12: “. . . for its resolution”. I suggest to remove these words, or replace by something like “. . . to achieve high accuracy”.

- p2, l12: “Adequate algorithms must then be used for its resolution”. I would expect a review of the literature on this topic at this location.

- p2: The four properties “conservation of mass”, “accuracy”, “positivity”, “flexibility” are generally considered in the context of solvers. Again, I would like to see a set of relevant literature references, and a brief overview of the available solvers, or classes of solvers.

- Introduction: What is the main motivation for developing a new solver? There are already a number of solvers readily available to choose from, which also satisfy a number of the properties mentioned. What are disadvantages of these other solvers, e.g. Rosenbrock, EB, twostep ?

- p3, l25: The second term on the left is diagonal. Please explain why ? Diagonal in which space?

- p3, l27: “mass conservation is not maintained”. Can you add a reference or text book? Is it possible to describe in one line how the reader may understand that there is no conservation of mass?

- p4, l8: Please name a few solvers that use this approach.

- p5, eq9: I guess an other requirement is delta_l,m = 1 - delta_m,l, which is fulfilled.

- p5, l27: Why is beta >= 1 required? Should this be beta > 0?

- p8, l6: if -> is

- p9, p10: Are the tables 1, 2, 3 really needed for this paper? Ref to Crassier and to the MOCAGE model description may be enough. The paper is already a bit long.

- p11, l2: “the ASIS solver gives acceptable solutions with less computation than the

higher order schemes." What the authors show is that the A1, which has comparable accuracy as R1 and G1, needs a smaller time step and more, but less complicated computations. In the end the effort is similar for the same accuracy. I do not think it is fair to claim "less computations than the higher order schemes", because this is at the expense of accuracy. Is it possible to relax the tolerance in the R1 and G1 schemes and to speed up these schemes in this way as well? Would this lead to similar performances as A2 or A3?

- Fig. 2: What is "H8CP" ? Also explain "PAN".

- P14, l4: damp -> use e.g. dampen, reduce, or diminish

- Fig.6. The colour scale is unclear: Does the colour between 1 and 2 mean there are two substeps or one substep? I assume "number of sub-timesteps" can only take integer values.

- p17, l16: "disequilibrium" Replace by something like "out of equilibrium"

- p19, l3: Replace "Figure 9" by "Figure 8"

- I find the discussion of Figure 9 a bit long. It is good to mention the large time step reduction in ASIS, and the figures speak for themselves.

- p22, l8: (Use of tendencies in the term F) I believe this approach has been used by e.g. Chimere. Adding emissions during the chemistry solver time steps has been used by more models. Please refer to this.

- p22, l29: Please add a reference for Euler backward.

- p23, l11: "mn" I assume you mean "minute"?

- p23, l13: ".. to ASIS in done .."

- p25, l32: "4 times smaller". How can I see this from the figure 12, which has a scale ranging between -30 to 30%?

- p28, “This objective can be achieved using multi-step high order algorithms but the computational cost of those schemes increases rapidly with the number of species considered.” It would be useful if the authors can make this point more explicit. How does the computational cost of ASIS compare with Rosenbrock as a function of the number of species. Perhaps the authors could introduce a figure to demonstrate this dependence.

- p28: I was wondering if ASIS could be used for adjoint (4D-Var) type of applications?

- p29, code availability: “The ASIS code is property of the CERFACS and includes libraries that belong to other holders.” Does this imply any restrictions if other parties want to use the code? Is there a kind of license for using the code?

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Discussion paper