

Interactive comment on “Numerical issues associated with compensating and competing processes in climate models: an example from ECHAM-HAM” by H. Wan et al.

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We thank Dr. Bonaventura for his helpful comments. Our reply is given below.

1) The description of scheme HAM1 should be more precise, it is unclear how the limiter is exactly implemented and whether the clipping acts on S^{} or on $S_{t+\Delta t}$ or on both. Furthermore, it is not clearly specified if the 95% limiting is also used in scheme 1EP. In general, it would be better to express all these limiting steps by formulae, including appropriate operators like $\max(S,0)$ in the definition of the numerical method.**

In the HAM1 scheme, a limiter is applied to S_{**} such that the amount of sulfuric acid gas
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condensed within one time step does not exceed 95% of S_* . A second limiter is applied to $S_{t+\Delta t}$ to avoid negative values. Both are used in scheme 1EP as well, to allow for a clean comparison between the sequential and parallel splitting of production and condensation. In the revised paper the limiters are explicitly included in the formulae (also for the other time stepping schemes), and clarified in the text.

2) The approach that leads to the method defined by equation 15 looks essentially equivalent to what is known in the literature on ODE solvers as the first order Rosenbrock or Euler-Rosenbrock linearized implicit method (see e.g. the book E. Hairer and S. P. Norsett and G. Wanner, Solving ordinary differential equations, Vol 2, Springer, 1987). If this the case, the proposed method should be referred to as a Rosenbrock method.

Eq. (15) in the discussion paper was derived by linearizing the aerosol nucleation term in the sulfuric acid gas equation around the initial concentration of a time step. This is indeed one of the key ideas behind the Rosenbrock methods. While the Rosenbrock methods also feature the use of multiple stages (thus are often interpreted as a type of Runge-Kutta methods), we use a single stage in the present paper. The focus is not an arbitrary order of accuracy, but rather the (large, first-order) error caused by operator splitting. Just like the Euler forward scheme is seldomly referred to as the one-stage Runge-Kutta method, we refer to our scheme as a linearly implicit method in Table 1 of the revised manuscript. On the other hand, following the referee's suggestion, the relationship between our scheme and the Rosenbrock methods is explicitly stated in Sect 2.2 of the revised manuscript.

3) The observation that splitting nucleation from other processes can lead to unrealistic results is contained in paragraph 27 of Jacobson 2002. It would be appropriate to acknowledge this indication, since the authors have referred to this paper anyway.

The following sentence is added to Section 2.2: “As pointed out by Jacobson (2002)

and shown later in Sect. 5 of this paper, solving nucleation together with condensation helps to correctly represent the competition between the two processes for the available sulfuric acid gas."

4) All the methods considered appear to be first order accurate as a whole. For clarity, some explicit comment on the order of convergence of these methods should be added.

The time stepping schemes used in HAM1 and HAM2 are both based on sequential splitting between nucleation and the rest of the ODE, which makes them first-order accurate. The schemes 1EP, 1Im and 2C are presented in the paper for the purpose of explaining the differences between the HAM1 and HAM2 results. Therefore they use the same sequential splitting between nucleation and production/condensation, and are also first-order accurate. This is clarified in Section 2.2 (below Eq. 10) of the revised manuscript. Scheme 3 in the discussion paper is first-order because of the Euler-backward discretization. This is also mentioned in the revised paper.

I understand that switching to a higher order method might not be worthwhile considering the overall efficiency constraints and that simple substepping might be more effective, but I believe that if the goal is to use long timesteps (actually, twice as long as those employed in the dynamical core) simple second order methods could also be useful. The authors might consider introducing a further test with a second order method, in order to check whether there is something to be gained by going higher order or not.

In the revised paper we added a "scheme 3A" which is similar to scheme 3 in the discussion paper (now referred to as "scheme 3B" in the revised manuscript) but applies the analytical solution of Eq. (12) instead of an Euler backward method. This scheme is essentially the exponential Rosenbrock Euler method, and is second-order accurate. As shown in the updated Fig. 2, the results are very similar to those from the original "scheme 3". This is not surprising because scheme 3 (now called 3B) already produces

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very small errors.

In addition, we would like to remark that in the global model, a time step twice as long as that of the dynamical core is employed not only for the sulfuric acid gas equation, but also for the whole physics package (except for radiation which is called every 2 hours). Since most of the parameterizations employ first-order integration methods, we do not expect to see a significant change in the overall results when using a higher-order scheme for the sulfuric acid gas equation alone.

5) For completeness, it would be interesting for the reader to show how scheme 3 performs in a box model test like that of Kokkola 2009. Reproducing something like fig.1 of Kokkola 2009 would be sufficient, possibly plotting the error with respect to the reference solution for scheme 2 and scheme 3.

Simplified tests as shown in Fig. 1 of Kokkola et al. (2009) are not included in the paper due to the consideration of representativeness. We find that the comparisons in our present work are more representative of situations encountered when running large-scale simulations than a limited number of box model comparisons.

Box model calculations were presented by Kokkola et al. (2009) for three cases of different parameter sets. Cases 1 and 3 were production-condensation dominating cases in which the role of nucleation was negligible, and the initial concentrations of the sulfuric acid gas were 1 to 2 orders of magnitude different from the corresponding equilibrium values. Such cases are, according to our experience, not typical in the ECHAM-HAM model. Also, because in both cases the sulfuric acid gas equation can be approximated to very high accuracy by the production-condensation equation, and the analytical solution of the latter is already exploited in HAM2, we expect the HAM2 scheme to give the most accurate results. Scheme 3 in the discussion paper would behave more like the Euler backward method in Kokkola et al. (2009), while the scheme 3A newly added to the revised manuscript would behave very similar to the HAM2 scheme. As for test case 2 of Kokkola et al. (2009), the aerosol nucleation plays a

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more important role. In such a situation, a comparison of the nucleation rates would be more informative than the H₂SO₄ gas concentration. In the manuscript, we present results of the sulfuric acid gas concentration as well as those of the condensation rate and nucleation rate, in terms of both global mean statistics and zonal-mean cross-sections, to reveal the performance of various numerical schemes in different regions and regimes in real-world simulations. We believe these are more informative for the model users than the box model calculations in Kokkola et al. (2009).

Reference:

Kokkola, H., Hommel, R., Kazil, J., Niemeier, U., Partanen, A.-I., Feichter, J., and Timmreck, C.: Aerosol microphysics modules in the framework of the ECHAM5 climate model – intercomparison under stratospheric conditions, *Geosci. Model Dev.*, 2, 97–112, doi:10.5194/gmd-2-97-2009, 2009.

Technical comments:

1) p. 687: stiffness is neither the only nor the most important issue addressed in the listed papers, this sentence could be reformulated referring more generally to numerical problems arising in this area.

“Stiffness problem” in the sentence is replaced by “the use of numerical techniques” in the revised manuscript.

2) p. 688 : Caldwell 2013 is missing in the reference list

The citation is changed into “Caldwell 2013, manuscript in preparation”.

3) p. 694 line 2: the authors claim that their ‘method 3’ is equivalent to a method proposed in Jacobson 2002, but the referred paper contains a large number of discretizations for different processes, it would help the reader to state specifically which formula in Jacobson 2002 one should look at.

The relevant equation and paragraph numbers in Jacobson (2002) are given in the

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revised manuscript. In addition, we added reference to Eqs. (16.68) and (16.74) of Jacobson (2005) for an easier comparison with our scheme 3 (“3B” in the revised manuscript).

References:

Jacobson, M. Z.: Analysis of aerosol interactions with numerical techniques for solving coagulation, nucleation, condensation, dissolution, and reversible chemistry among multiple size distributions., *J. Geophys. Res.*, 107, 4366, doi: 10.1029/2001JD002044, 2002.

Jacobson, M. Z.: Fundamentals of atmospheric modeling, Cambridge University Press, 2nd edn., 2005.

4) The stability analysis in appendix A is very standard and can be omitted, referring instead to some basic numerical methods textbook.

The stability analysis is removed from the paper. We refer instead to Chapter 2 in the book of Butcher (2008):

Butcher, J. C.: Numerical methods for ordinary differential equations, John Wiley & Sons Ltd., 2nd edn., 2008.

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