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Atmospheric Chemistry and Physics Discussions

Interactive comment on "Technical Note: The new comprehensive atmospheric chemistry module MECCA" *by* R. Sander et al.

R. Sander et al.

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We have revised our ACPD paper according to the suggestions of the referees. Also, we have included a few bug fixes in the code and updated the electronic supplement accordingly.

Referee 1:

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> Thus it might be helpful to discuss the problem of the
> numerical solvers in one or two more sentences (a detailed
> description is beyond the scope of this paper, the reader
> should refer to the well written paper by Sandu et al.
> (1997)). To me, the important problem of solving stiff
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> equation systems remains somewhat unclear. The authors
> emphasise the need for solvers with automatic time step
> control, which I understood. When introducing the
> Rosenbrock solver they mention schemes of second and third
> order. Are third order solvers needed for stiff equations?
> Or is it sufficient to have the automatic time step
> control? Are Rosenbrock second order and automatic time
> step control exclusive? A short clarification would be
> fine.

Both, the second and third order solvers can be combined with either automatic or manual time-step control. The KPP package includes a second order Rosenbrock solver with automatic time-step control (ros2-auto) which was not mentioned in the text. We found that the differences between ros2 and ros3 are relatively small when automatic time-step control is used for both. The third-order solver was faster for our chemical system, so we use it as default. However, we have not systematically analyzed the differences. We agree that it is necessary to refer to other literature like Sandu et al. (1997) if detailed information about the properties of the different Rosenbrock integrators is needed.

Referee 2:

> As for the scientific merits of the package, a detailed
> investigation of the properties of the solver is beyond
> the scope of the paper but would certainly be needed in
> future publications. Two such papers are already announced
> by the authors. The two examples of MECCA in use are
> encouraging but more will be needed.

We agree. We have only listed the two papers that we have planned next. In

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addition, there will be several follow-up papers on miscellaneous aspects of atmospheric chemistry by colleagues who have already started to use MECCA at other institutes (e.g.: DLR Institute of Atmospheric Physics, Oberpfaffenhofen, Germany; Forschungszentrum Karlsruhe, Germany; University of Crete, Greece; York University, Toronto, Canada; Beijing University, China).

> Also perhaps some more explicit discussion of other
> solvers, some of which are also freely available and use
> similar approaches to turn chemistry into code, should be
> in order.

We have now listed several other numerical software packages in the section Numerical flexibility and also explained why we have selected KPP.

> I found one problem in the supplement listing the chemical
> mechanism. Reaction G3107, according to Sander et al.
> (2003), produces N2O + O not N2 + O2.

Thanks. The error has been corrected in the equation file.

Interactive comment on Atmos. Chem. Phys. Discuss., 4, 7167, 2004.