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Atmospheric Chemistry and Physics Discussions

Interactive comment on "Technical note: application of α-QSS to the numerical integration of kinetic equations in tropospheric chemistry" *by* F. Liu et al.

Anonymous Referee #1

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General comments

This paper applies a numerical integration method previously used for combustion studies to tropospheric chemistry modelling. The authors use box model studies to illustrate the performance of the technique. A strength of the paper is the use of two different chemical mechanisms in a range of scenarios to illustrate the performance of the alpha-QSS method. There is also a good description of the accuracy and computational performance of the method.

There is insufficient new results presented in this paper to be a normal ACP submission

and the authors submit it as a technical note. However, as such, the purpose of a technical note would be allow prospective users of the scheme to decide whether to use it and advise on its performance, configuration and implementation. In this regard the paper has a number of shortcomings that are detailed below. However, work on improving integration methods is very welcome and continues to be very important for existing and new chemistry climate and transport models.

Specific comments

It is disappointing that the authors only describe box model studies in this note. Whilst such studies are a necessary step in implementing and evaluating a new integration scheme it does not follow that the scheme will be efficient in a three-dimensional climate or transport model which potential users will need to know when reading this paper. For example, stiff solvers in 3D models such as the SMVGEAR methods of Jacobson use sparse matrix methods and rearrangement of the grid nodes to achieve efficiency. Whilst it appears from the work presented here that the alpha-QSS scheme should be straightforward to implement in 3D it is NOT obvious it will be efficient or competitive compared to other integration methods currently used. For example, Fig. 10 shows that there is a significant difference in the cost of the scheme and variation of cost with efficiency depending on the chemistry being solved. In a 3D model, there will obviously be a mix of chemical scenarios being solved simultaneously. The authors should comment on implementation of the scheme in a 3D model and any issues they expect to need to address. Given the highly parallel nature of todays atmospheric models and importance of optimisation on computer hardware, it would also be useful to have some short comment on aspects such as vectorisation of the code, whether communication costs would be required for an efficient parallel implementation and so on. I suspect these would probably not be issues for the alpha-QSS method, but they are questions which arise when considering implementation in 3D atmospheric chemistry models on high performance computers.

Another shortcoming of the paper is the use of only the VODE integrator for compar-

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ison. The authors do not state whether they have used the 'off-the-shelf' VODE code from NETLIB (for example), whether they supply VODE with the Jacobian matrix or whether the VODE code computes it as a finite difference, whether they have modified VODE to use sparse matrix methods to invert the Jacobian. These can significantly alter the cost of the VODE code and without more details it is very difficult to assess the performance of the alpha-QSS scheme. The authors need to be more specific on how the VODE integrator is being used.

It would greatly improve this paper if the authors could compare their method to one currently used by 3D models, possibly repeating a comparison study published previously. The work of Sandu and colleagues would be one example.

I'd also suggest longer integrations to see whether the alpha-QSS method introduces any bias or trends in the time evolution of key species such as ozone compared to VODE or other integrators.

Section 3. When the authors introduce the parameter alpha, they do not explain why it takes this particular form, only noting that it differs from previous methods. There should be some description of why this form is used; is it more accurate, lead to faster convergence than previous QSS methods? A citation here to the relevant publication giving more details would also be useful.

One suggestion I would like to make is whether the authors would consider making the code for their scheme available to download on the internet (perhaps under an open-source license agreement). There are a number of integrators available in this way.

The list of publications cited by the authors is fairly comprehensive. However, two comments: first avoid the use of publications which are technical reports as these can be very difficult to obtain, second the authors might wish to reference the SMVGEARI &II methods (as used in the GEOS-CHEM CTM) as these are well respected integrators.

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There are rather a lot of figures accompanying this note. I would suggest that figure 1 is not necessary. The parameter alpha is adequately described in the text. Perhaps in figs 3 & 4 only one of the NO/NO2 figures needs to be shown?

Typographical comments

The paper needs to be read for grammar. There are a number of sentences that need to be rewritten. For example, the first sentence of the introduction would read better as : Comprehensive atmospheric chemistry transport models (CTMs) have been developed to improve understanding of the transport and fate of trace gases and pollutants in the atmosphere. The sentence at line 16 of the abstract starting 'This comparison..' is another example.

Abstract line 10. The phrase 'testing results' is used throughout the paper. This should be 'test results'.

Section 2. Line 20. Carbon Bon Ĕ is missing a 'd'.

Section 3. eqn 10. The use of subscript 'P' is perhaps a little confusing with the chemical production 'P'. A different symbol/letter should be used.

Fig. 9. The RERR O3 plot only shows 3 curves. The one for epsilon = 0.10 appears to be missing.

Fig. 10. The y axis has no numbering.

Interactive comment on Atmos. Chem. Phys. Discuss., 5, 6215, 2005.