Atmos. Chem. Phys. Discuss., 5, S2674–S2676, 2005
www.atmos-chem-phys.org/acpd/5/S2674/
European Geosciences Union


Atmospheric Chemistry and Physics Discussions



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

**Anonymous Referee #2**

Received and published: 16 September 2005

General comments.

The paper presents the comparison of a QSSA based numerical ODE solver CHEMEQ2 against a more traditional VODE based method for applications in tropospheric chemistry. The purpose of the paper should therefore be to provide useful information to readers to enable the selection of the most appropriate integration tools for particular problems in tropospheric chemistry. To this end the scenarios chosen and chemical mechanisms used seem to be appropriate. The scenarios follow well documented cases introduced by Poppe et al. that cover a wide range of conditions.

The use of full and reduced chemical mechanisms allows a useful comparison of the impacts of lumping on the predicted concentrations of important species. However, the comparison with only the VODE integrator to my mind is problematic for several reasons that will be outlined below.

Specific comments.

There has been a huge amount of previous work carried out by talented numerical mathematicians over the past decade comparing fast solvers for atmospheric chemistry problems. The work of the group of Verwer and coworkers and Sandu, Carmichael and coworkers has been extremely valuable in providing comparisons for a wide range of simulation scenarios. In particular, the two review papers of Sandu et al. that appeared in Atmospheric Environment vol. 31 (these papers would be a much better reference than the technical report referred to here) to a certain extent set the bench mark for comparisons of efficiency of solvers. These two review papers covered more than 10 integration schemes and several tropospheric, stratospheric and urban scenarios.

The first point of relevance to the current paper is that Sandu et al. showed in 1997 that the efficiency of the VODE method is very sensitive to the method used for the exploitation of sparsity. In order to class as more efficient than VODE based methods then it is important for the CHEMEQ2 method to be compared against a sate of the art VODE solver that uses appropriate exploitation of Jacobian sparsity. I could find no mention of sparsity with respect to the VODE method in the paper or in the reference cited for the VODE method used. In my view this is a significant problem that needs to be addressed. If the VODE method used for comparison does not exploit sparsity then the comparison is not a fair or useful one.

In addition, the work of Sandu showed that the VODE method was efficient when high accuracy was required but that Runge-Kutta_Rosenbrock and 2-step BDF type methods could be much more efficient for lower accuracy solutions for a wide range of scenarios. In my view therefore, in order not to give a misleading impression of the ef-



**ACPD**

5, S2674–S2676, 2005

ficiency of the CHEMEQ2 method, it should be compared against at least one Rosenbrock type scheme as well as the most efficient VODE scheme. In one sense the 2-step method could perhaps could be avoided since it is not generalisable to wet applications and has been compared against Rosenbrock and VODE schemes by Sandu et al.. It may well be that the CHEMEQ2 solver stands up well to such comparisons but this is certainly not clear from the work presented here. I am not a numerical mathematician and purely a user of numerical integration schemes. From my point of view if a new solver is to be considered for use I would like to see it compared with the "best of the rest". Without the kind of full comparison, as introduced by the work of Sandu, Verwer and others it is difficult to form a clear opinion about whether to use the solver presented here, as well as how it fits in with previous work.

Typographical errors.

P6226 line 11 apecies -> species

There seems to be no scale on the y axis in figure 10.

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