Geosci. Model Dev. Discuss., 2, C185–C187, 2009
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Geoscientific
Model Development
Discussions

Interactive comment on "Automated sequence analysis of atmospheric oxidation pathways: version 1.0" *by* T. M. Butler

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Received and published: 25 August 2009

Many thanks to the reviewer for their positive comments on the manuscript.

The reviewer makes the point that the sequence method is not well enough described. As well as a detailed description of the algorithm in Section 2 of the manuscript, I believe the text at the beginning of Section 2 describes the method quite succinctly.

> The basic idea behind the algorithm is to start at a "root species", and determine its oxidation products and the side effects of its oxidation reactions. Each of the oxidation products is then treated as an intermediate product for which the process is repeated.

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Interactive Discussion

Discussion Paper

On the other hand, perhaps the manuscript could benefit from a more explicit description of the oxidation sequences of CH_4 in the introduction. I would propose to add some text to the introduction, specifically to the description of the work of Johnson and Kinnison (1998). Perhaps I could fully describe one of the possible CH_4 oxidation sequences (along with the side effects on radicals) to make it clearer what is meant by an oxidation sequence.

I agree with the reviewer that it would be less confusing if the text were to refer to the total rate of chemical destruction of the root species, rather than the rate of production. I propose to change this in the revised manuscript.

Regarding the memory and CPU performance of the algorithm, this is highly dependant on the implementation. The sample implementation in in the electronic supplement is written in a dynamic programming language (perl5) which would in general be expected to use more CPU time than an implementation in a compiled language (such as C or FORTRAN). On the other hand, the sample implementation makes use of hash tables (or associative arrays) to store much of the information. This takes advantage of the sparseness of the system (eg. not every reaction influences every chemical species in the system). An implementation using simple two dimensional arrays (as represented in the pseudocode version of the algorithm in Figure 1 of the manuscript) would use considerably more memory. As the reviewer also points out, the performance of the algorithm also depends on the root species chosen and the value of $min\_fraction$ used. Instead of going into too much detail about this in the revised version of the manuscript, I propose to add some text briefly stating that the performance is dependant on the implementation, the input parameters, and also on the complexity of the chemical mechanism.

There is no reason why the value of 1×10^{-9} should be low enough to allow the sequence algorithm to converge in all cases. A test for convergence would be a good idea for a future version of the algorithm, as suggested by the reviewer. This would save the user from the need to manually check this.

GMDD

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Interactive Comment

I agree with the reviewer that perhaps it goes slightly too far to claim in the present manuscript that the use of the sequence algorithm represents an alternative to traditional methods of calculating ozone production potentials. I propose to tone this down somewhat by changing this to "...potentially represents...".

Interactive comment on Geosci. Model Dev. Discuss., 2, 1001, 2009.