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Discussions

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

Anonymous Referee #2

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1 General comments

This paper presents a new automated method to analyse the output of photochemical models. The algorithm is described and its use illustrated with a series of applications of increasing complexity. Overall the algorithm is clearly and concisely explained. The results provided demonstrate that the algorithm gives the expected results for those test problems where the results can be derived from inspection of the photochemical model output. In the case of NO2 production by VOC it is demonstrated that the results are consistent with what would be expected. This method offers a new way to gain scientific understanding by better exploring the results from photochemical modelling.

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2 Specific comments

I have a few fairly minor comments. It would be worth explicitly defining what is meant by the sequence method - at present this is only done implicitly by describing the early work.

In section 2 para 2 it states "initially called with the root species and the total rate of production of this root species". This is confusing as one normally considers many VOCs as being destroyed by the chemistry rate, although in the experiments described here where the concentration is held constant of course in effect production is forced to equal loss.

It would be worth commenting somewhere on some typical times taken to run the algorithm and memory usage (with the simple code attached, it only takes a few seconds to run on my PC, but does depend significantly on the value of min rate chosen and there is a difference between solving for CH4 and HCHO).

On choosing a value of min_rate, section 3 states that a value of 1x10-9 is sufficient to ensure that the uncompleted reaction sequences can be ignored but it is unclear if this is specific to the mechanism being analysed or more generally true. If this is not generally true, might it be worth adding code to iterate the sequence mechanism and test for convergence? (This would probably something for a future version however and is certainly not needed for the work to be published)

Finally, in section 5 the statement is made that "the SEQUENCE algorithm represents an alternative method for the calculation of ozone production potentials". I am not convinced that the results presented in this paper are sufficient to justify this statement - it is noted later on that to fully demonstrate this several other factors need to be accounted for. What has been demonstrated here is that the algorithm can calculate NO2 yields from VOC oxidation. I look forward to the follow up paper on this topic.

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