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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

I was not aware of the previous work by Tonneson, and I thank Barron Henderson for pointing out this work. The "history matrix" approach does indeed seem to be a related technique, inasmuch as this technique and the sequence approach are both intended to calculate the effects of individual VOC on species such as NO_2 and OH. The existence of this previous work warrants a reference to the PhD dissertation of Tonneson (1995) in the revised manuscript.

While the sequence method starts at a VOC of interest and follows the reaction sequences leading from this VOC through its intermediates to its end products, producing a list of affected species, and for each of these affected species a list of production and loss reactions which are ultimately all attributable back to the original VOC, the history

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matrix method appears to focus foremost on the intermediate (or "replaced") species themselves. If I understand correctly, the history matrix method ultimately builds up a picture of which emitted VOC contribute to the mixing ratio of the replaced VOC. In order to determine this kind of information using the sequence method, the method would need to be run individually for each emitted VOC to determine the production rates of each intermediate. Conversely, in order to determine the effects of each emitted VOC on each on their affected species using the history matrix technique, the effects of each of the production and loss reactions of each of the replaced species must be summed (along with any effects of the reactions of the emitted VOC themselves) and weighted by the contribution of each emitted VOC to each replaced VOC.

An interesting difference between the history matrix approach and the sequence approach is that the former keeps track of the initial mass of chemical species, and follows the time steps in the photochemical model, while the latter analyses a single set of reaction rates. The history matrix approach produces a time-dependant result when run with reaction rates from multiple model time steps, while the sequence approach produces an averaged result when run with averaged or steady state reaction rates. This shows up an important limitation of the sequence approach: when the chemical rates used for the calculation include the presence of initial mass of intermediate oxidation species (or excess production from a previous model timestep), then the chemical loss of these intermediates may be greater than the chemical production due to the precursors. This will result in mass being added to the middle of the sequence, and may inflate some of the calculated influences. No previous applications of the sequence algorithm have suffered from this problem due to the use of appropriately chosen reaction rates. It is however necessary to mention this limitation of the approach in the revised manuscript.

Regarding automatic loading of the reaction rates and stoichiometry, yes, this has been done. I chose to hard-code this information in my online supplement because the code which reads this information is heavily dependant on the particular model input and

output file formats used in-house. A fully generalised set of input gathering routines is beyond the scope of the current (proof of concept) manuscript. I believe that the approach I have adopted exposes the details of the algorithm to a high enough degree to enable interested users to code input routines applicable to their own file formats.

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

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