Geosci. Model Dev. Discuss., 2, C140–C141, 2009
www.geosci-model-dev-discuss.net/2/C140/2009/

Geoscientific
Model Development
Discussions

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

B. Henderson

barronh@gmail.com

Received and published: 4 August 2009

This technique sounds very similar to the History Matrix technique. The history matrix technique was developed by Tonnesen in 1995. The technique is detailed in Tonnesen's dissertation Appendix C. For convenience, I have attached that dissertation cover page and Appendix C as a supplement.

The Tonnesen approach uses a differential equation to account for production and loss. The differential approach is important to account for different loss rate of chemical mass produced during the analysis compared to pre-existing mass (see Equation 2 of Appendix C). If I read your code correctly, you are using an algebraic yield instead.

Can you comment on how your work differs from or is similar to Tonnesen's? Also, can

you comment on how important you expect the algebraic yield to be? Finally, have you looked into automatically loading the reactions and stoichiometry?

If you are interested in reviewing Tonnesen's Fortran code, it is available at the following URL: https://dawes.sph.unc.edu/trac/pyPA/browser/tags/fortran-with-branches/irr/trunk

Please also note the Supplement to this comment.

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

GMDD

2, C140–C141, 2009