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Atmospheric Chemistry and Physics Discussions

Interactive comment on "Development of a simple unified volatility-based scheme (SUVS) for secondary organic aerosol formation using genetic algorithms" *by* A. G. Xia et al.

WRS Stockwell (Referee)

william.r.stockwell@gmail.com

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Overall the paper has much that is new and interesting. This paper will be very useful to those trying to implement the chemistry of secondary aerosol formation in air quality models and to link it's formation with gas-phase atmospheric chemistry mechanisms.

The authors have developed a "simple" scheme to describe the formation of secondary organic aerosol based on a binned approach with 312 stochiometric coefficients and 100 reaction rate coefficients. They used the Master Chemical Mechanism.(MCM) to generate many atmospheric cases. A new approach based on genetic algorithms was used to set the 412 coefficients by fitting the MCM generated cases. This application of

genetic algorithms to fit the data is very interesting and this method should have further applications in atmospheric chemistry. However there will be a steep learning curve for most and a high computational investment required.

The paper addresses several problems in the current volatility-based set (VBS) approach for modeling the formation of secondary organic aerosol. The first problem is that the VBS approach treats the formation of secondary organic aerosol as a one-step process. While VBS may fit reaction chamber data is likely that aerosol formation will occur over much longer time-scales in the real atmosphere. Atmospheric oxidation of higher molecular weight organic compounds involves several reaction cycles of their products that will occur over an extended time period. However it is difficult to treat this complicated secondary organic chemistry because there is a high uncertainty in the product yields. Not only are the yields as determined from fits of data are uncertain but also they depend on atmospheric conditions. An approach that involves a more explicit treatment of the chemistry is needed although many uncertainties will remain.

The main concern is that the validity of their scheme is limited by the validity of the Master Chemical Mechanism. While the MCM has considerable detail it is far ahead of the experimental data. Although the MCM is a very worthy effort, much of it is built from estimates, extrapolations and mechanistic analogies based on the limited available laboratory data. The authors almost reach an important point in that the MCM is rather artificial in the sense that it treats the products all the way from the "initial oxidation step to the final products, CO2 and H2O". Actually the authors' results depend on a fraction of the products condensing out of the gas-phase and not participating further in the MCM gas-phase chemistry.

Another concern is that the final result is a highly parameterized fit. Although the fit may be sufficient for modeling it does not appear to provide much insight into the real atmospheric processes that scientists what to understand. Maybe the authors would want to comment on this point.

But paper remains an interesting and helpful contribution to the literature.

Interactive comment on Atmos. Chem. Phys. Discuss., 11, 3885, 2011.