

Interactive
Comment

Interactive comment on “An extended secondary organic aerosol formation model: effect of oxidation aging and implications” by F. Yu

S.L. Napelenok

napelenok.sergey@epa.gov

Received and published: 7 October 2010

This is an interesting and well written manuscript on an enhancement to the $n \times 2p$ model for SOA formation and its implementation in the GEOS-Chem model. Some comparisons with observations are provided at a boreal site in Finland and several implications for climate forcing calculations are discussed.

I have reviewed this manuscript with several colleagues at EPA and we came to a consensus at offering the following questions and recommendations centered mainly on model formulation:

The majority of new SOA papers coming out currently are some kind of an extension to existing models, so it may be beneficial to come up with a title that uniquely distin-

Full Screen / Esc

Printer-friendly Version

Interactive Discussion

Discussion Paper



guishes your work from other “extended SOA models.” In the text, perhaps you can build upon Jim Pankow’s $n \times 2p$ nomenclature (e.g., use “ $n \times 2p$ + SOG” aging instead of just the word “extended”).

When the terms SV-SOG and MV-SOG are introduced in the Abstract, it would be helpful to provide the range of c^* values that these two groups span at 290K.

It may be beneficial to clarify your reasoning on why particle growth should be modeled kinetically rather than thermodynamically (page 19815, line 16).

How appropriate is it to age an Odum 2-product model given that the Odum 2-product model may overpredict the amount of gas-phase SOG? For example, Cappa and Jimenez (2010, ACP) found that the amount of semivolatile gas-phase organic in equilibrium with OA could range from 20% to 400% of the OA mass with smaller values generally corresponding to higher (and perhaps more reasonable (Epstein 2010 ES&T)) enthalpies of vaporization.

Donahue’s parameterization of the enthalpy of vaporization (page 19817, line 10 – 11) was recently updated (see Epstein et al., ES&T 44:743-748, 2010). Perhaps a column of ΔH_{vap} values can be added to Table 1.

The standard distribution of compound vapor pressures was likely chosen as a mathematical convenience, but is there any evidence to support this assumption? From the caption of Figure 3, it seems that the standard deviation of 2 was used in the analysis. It would be helpful if this was stated in the text along with some explanation of how was this parameter was determined and under what conditions it might be different.

Are equations (6) – (8) solved by operator splitting? If so, in what order are the processes of partitioning, nucleation, and oxidation solved?

Do the new and existing aging/oxidation reactions consume radicals in the chemical mechanism?

What deposition and scavenging parameters are assumed for each SOG species?

C8395

Full Screen / Esc

Printer-friendly Version

Interactive Discussion

Discussion Paper



It seems that only 6 additional tracers were added to the model to accommodate the mechanism enhancements (page 19821, line 27). I understand that the different size bins were tracked as an aggregate and split when necessary based on surface area. However, it is not really clear how it was possible to track the first generation products for all the species coating the several listed surfaces (dust, poc, etc.)

In the manuscript you frequently use the term “vapor pressure.” You probably really mean “saturation vapor pressure.” If that is the case, it should be changed for clarity.

In equation (8), why is only condensation but not partitioning included for a loss pathway of LV-SOG (i.e. why is there no L_{par} term)?

Page 19818, lines 14–18: The authors use a new term HV-SOG without defining it. Based on their C^* values (10 ppb – 10 ppm), does HV-SOG include VOC1-6? Or are the HV-SOG analogous to Robinson’s IVOC? It might be useful to make this connection.

Page 19820: What is the C^*_{upp} for LV-SOG based on?

Page 19821: It would be helpful to give a few details about the PM sectional size distribution. How many bins are used?

Figure 5: The text states several times that this figure “clearly” shows improvement from the no oxidation case to the oxidative aging case when comparinnig to observations. To me, this figure is not very clear at all. Is there a better way to present this? Perhaps show “difference” plots between the two cases and observations?

Figure 8: Reporting NME and NMB values for the data in this figure would help to quantify the improvement. It would be helpful if the results of this model application were placed in context with other recent efforts to extend the SOA treatment in GEOS-Chem (e.g., Pye & Seinfeld) and regional scale models (e.g., biogenic SOG is not aged in PMCAMx). On line 1 of page 19815, please replace the reference to Schell et al. with (Carlton et al., ES&T in press).

[Full Screen / Esc](#)[Printer-friendly Version](#)[Interactive Discussion](#)[Discussion Paper](#)

Interactive comment on Atmos. Chem. Phys. Discuss., 10, 19811, 2010.

ACPD

10, C8394–C8397, 2010

Interactive
Comment

Full Screen / Esc

Printer-friendly Version

Interactive Discussion

Discussion Paper

C8397

