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Atmospheric Chemistry and Physics Discussions

Interactive comment on "A Functional Group Oxidation Model (FGOM) for SOA formation and aging" *by* X. Zhang and J. H. Seinfeld

Anonymous Referee #1

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The paper presents a new simplified, yet flexible, model of SOA formation based on empirically fitted parameters. Sensitivities to processes are modeled by varying parameters within the fixed model framework. In all, the paper is quite interesting in that it assesses the ability of another semi-empirically formulated approach to understanding SOA formation. It is suitable for publication in ACP when some general issues have been addressed. Overall i would recommend more references are given to support various statements throughout. A few are mentioned below.

General comments: The authors raise an interesting point, that being the trade-off between chemical fidelity and computational feasibility. I agree that the drive to include accurate SOA models in large scale schemes is critical. With this in mind it must also not be forgotten that the role of the more complex mechanistic approaches still holds

for increasing our basic understanding of important aerosol processes. In the drive for developing reduced complexity models for use in large scale sensitivity studies, this parallel ethos must be maintained. Do the authors have a feel for which processes that might be occurring in real-world aerosol, that are not accounted for in this model, that might lead to biased sensitivities derived using this framework?

One important statement is made at the beginning of the document. The authors state how 'laboratory chamber data on which current models are based generally do not exhibit the degree of oxidation observed in atmospheric organic aerosol'. If we are left with models that have to be tuned to such environments, it is then dangerous to prescribe 100% confidence in subsequent sensitivity studies for real-world scenarios? This is a harsh question perhaps, but with the rise of the tuned semi-empirical model that the authors concisely review, it is useful to think about this.

There are numerous assumptions made in the inclusion of specific processes such as fragmentation. As the model is then fit to experimental data, do the authors have any mechanism for testing the sensitivity to these assumptions before even the sensitivity of the process??

Minor comments.

Page 32569. 'This is in contrast to the fully explicit chemical model that has, in principle, no adjustable parameters'. On the contrary, the flexibility of parameter adjustment is huge in the 'fully explicit models. Whilst often sold as a 'black box' there is much scope for testing, for example, the importance of specific reaction pathways. Or are the authors referring to something specific such as a process level phenoema?

Page 32573. I don't think the statement that 'a combination of these four groups is assumed to be a sufficient surrogate for all functional groups in terms of the contribution to vapor pressure..' is technically correct. There is a large body of work on the correlation between vapour pressure and specific functionality. If referring to very simplified predictive techniques, that don't actually perform very well for a large subset of atmo-

spheric organics, this should be stated. Also, please add more supporting references in this paragraph.

Page 32575: What is a 'Hockey Stick' in the O:C vs C* space? Is there a figure to refer to or can I assume something L-shaped?!

Page 32576, line 20. In what way advantageous? Easy to use? Equation.2 Where has this equation come from?

Page 32577. Line 27. This isn't correct, if using mole fractions the activity coefficient should be on a mole fraction scale not molality based (1 for the pure liquid). Also, please refrain from placing equations in line with the text.

Section 3. What boundaries are placed on the fitted variables?

Page 32585, line 6. Please state and reference range for which 'AMS measurements are less reliable'.

Interactive comment on Atmos. Chem. Phys. Discuss., 12, 32565, 2012.