Geoscientific
Model Development
Discussions

Interactive comment on "The Secondary Organic Aerosol Processor (SOAP v1.0) model: a unified model with different ranges of complexity based on the molecular surrogate approach" *by* F. Couvidat and K. Sartelet

Anonymous Referee #1

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The Couvidat and Sartelet manuscript reports on a flexible model (SOAP) for predictions of secondary organic aerosols (SOA) intended for use in three-dimensional air quality models. The availability of a flexible SOA model is attractive and would represent a novel contribution to the field. However, it is recommended that the manuscript be significantly improved before being published in GMD. The manuscript has weaknesses in overall language and fluidity (presentation quality), as well as proper citation of related work (scientific quality). There are also a few specific scientific quality questions to be addressed. Details of these areas needing improvement are provided

below.

Presentation Quality: It is recommended that the authors carefully review the language in the manuscript and if necessary, request the assistance of an additional reader/editor. In many places it seems errors may be due to carelessness and thus the latter would not be required. For example, condensation or absorptive partitioning describes dissolution of a gas-phase species into a particle; throughout the manuscript the authors discuss condensation "on" or "onto" aqueous and organic phases/particles. In a few places the authors correctly describe condensation into the aqueous and organic phases/particles. It is important to distinguish these processes because partitioning on/onto a particle surface is also important in the atmosphere, but not the subject of this manuscript. A few more examples follow, which are relevant for interpretation and reproduction:

p. 385, line 10: The authors discuss the need to account for inorganic aerosol formation "previously". Do they instead mean separately? Or concurrently? Also, the authors should provide a complete list of the SOAP inputs from ISOROPIA, rather than a partial list as indicated by "such as".

p. 405, line 3-7: It is not clear what the authors mean when they write that "As in H2O, some species do not have a molecular structure attached. . .". "However, . . . is taken into account using a default molecular structure as in H2O." Do they mean that while molecular structures are specified for some surrogates, the others are defined by a single default structure? Is that structure the same for each surrogate (which seems problematic given the range of surrogates listed for which there is no molecular structure)? If it is not the same for each surrogate, how is a default structure for each surrogate different than a molecular structure?

The abstract lacks discussion of results. Inclusion of some statistics on the relative performance and computational time of the various model configurations is recommended. The authors may want to consider putting some of the developmental equa-

tions in supplementary material. For example, equations 1-7 are well known and may not be needed. Equations 17-19, 22, 24 describing partitioning to an aqueous phase are analogous to equations 14-16, 21, 23 for partitioning to an organic phase; one set could be moved to a supplement, with the differences described in one or two sentences. (e.g., "Analogously, partitioning to an aqueous phase can be represented by equations x, y, z, where $K_{p,i}$ is replaced by $K_{a,i}$...".)

There are multiple instances in which the authors mention "several" particulate phases; however, the manuscript details consideration of up to two phases only.

Scientific Quality: The authors introduce a number of model approaches in which one or more of the considerations discussed in the manuscript have been taken into account. The authors miss an important publication in which phase separation and partitioning kinetics have been considered: Shiraiwa et al. (2013), Phys. Chem. Phys., 15: 1141. Relatively few references appear in the methodology, for example previous model approaches for phase separation (e.g., Zuend and Seinfeld, ACP, 2012; Erdakos and Pankow, 2004). The results are not put in the context of existing work considering non-ideality, phase separation, and kinetic partitioning (including the influence of RH on equilibrium timescales, see for example Saukko et al., 2012; Renbaum-Wolff et al., 2013).

p. 381, line 6: Total particulate mass? Or total fine particulate mass?

p. 382, line 3-5: It is not clear what the authors mean when they discuss separation of organic matter into several phases due to saturation.

p. 384, line 18: The authors state that saturation vapor pressure is usually determined experimentally. However, the manuscript is describing a molecular surrogate approach, thus experimentally determined vapor pressures would not be available. It would be more appropriate to describe the approach for obtaining the saturation vapor pressures for the molecular surrogates.

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p. 386, line 6: Does "AQ" include water?

p. 386, line 16: The authors state that UNIFAC only accounts for short-range interactions. This is not accurate. See for example Erdakos et al., 2006. Furthermore, it isn't clear why the authors don't just use AIOMFAC for the short-range interactions as well.

p. 387, line 18-21: It isn't exactly clear why SOAP would predict less water than the inorganic model, assuming that total water is "organic water" + "inorganic water", and the inorganic water is used as an input to Eq 13. The authors should expand/clarify this point.

p. 387-388: Given that each molecular surrogate has some fixed properties, it isn't clear why the user would want to specify hydrophilicity/hydrophobicity, unless there is an option to add structures, which is not discussed in the manuscript. The flexibility to consider partitioning to one or both phases is appealing, but when the "both" option is turned off, it seems that each structure would simply have an assigned preferred phase.

p. 394-395: The authors describe the use of $P_{eq,i}$ instead of saturation vapor pressure to account for the Kelvin effect (equations 41, 45); however, $P_{eq,i}$ is not the Kelvin-corrected saturation vapor pressure (as suggested by Eq 41) which is the correct substitution in Eq 45. See for example Pierce et al., 2011.

p. 408, line 6-7: What is the rationale for chosen accommodation coefficient and gas-phase diffusion coefficient?

Editorial (these are a few examples, many others exist): Section 2.1, p. 382, line 24/25: "has been developed" not needed p. 383, line 4: "process" should be "processes" p. 409, line 11: sp. "measuremeants"

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