

**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"**

### **General Comments:**

It is still not apparent to me why assuming the independence of the relationship between each layer and the gas-phase is acceptable. The authors assert this fact and express it in plain form (Eqn. 52 and 53), while also stating that overcoming it will be the subject of future work. There may be something to the underlying mathematics and scaling that makes the assumption reasonable, but, if so, I don't see it. More work with the model and other applications will bear this out. In the meantime, assumptions like this one make the methods section difficult to follow, as described below. For instance, it is hard to swallow the uniform application of the Kelvin effect term on each individual layer in Eqn. 53; it is equations like this that give the reader pause and interrupt the flow of the manuscript.

I appreciate the extra work the authors have put in to improve the presentation quality, model description, and discussion of results. Unfortunately, I think it is still a generally confusing manuscript (specifically parts of section 2.3). The language used is rather wordy in places and somewhat imprecise in others. The level here would normally be acceptable, but the assumptions and complexities of this particular model application make it extremely important that every word is as precise as possible. I am willing to recommend this paper for publication after the issues below are addressed.

### **Presentation Issues:**

1) Section 2.3.3 is extremely difficult to understand. After reading it three times, I am still having a hard time following the subscripts and pluses and minuses. If there is any way to clarify the presentation, maybe with the addition of a cartoon illustrating the relationships among the various fluxes and factors, I would recommend adopting it. Part of the problem, I think, is that the authors are suspending, as they state, some laws of physics in order to make the simplifications they desire for efficiency. It then becomes hard to remember, for instance, which summations are happening over bins (Page 21, line 6) and which are over layers (Eqn. 52). The authors attempt to explain why local fluxes for specific layers can be ignored when they are opposite in sign to the global flux (Pages 22-23), but this explanation is also somewhat lost in nomenclature and subscripts. I repeatedly missed the essence of the argument.

Sentences like that on Page 23 (Lines 2-5) are generally confusing, “The total flux of... is separated into *two* fluxes...” yet there are three fluxes on the right hand side of equation 56. Why is the statement on Page 23 (Lines 13-17) true?

2) The equilibrium timescale,  $\tau_{eq}$ , is defined with respect to a specific bin, layer, and species (Eq 75), but then in Sections 2.3.9 and 2.3.10, it is applied with reference to ‘cases’. Are these ‘cases’ just specific combinations of bin, layer, and species volatility, or are the equilibrium/dynamic option applied globally. How much control does the user have? What error is introduced in Eq. 83 when only the mass at equilibrium is counted in the ‘ratio’ variable? Why isn’t all of the material (equilibrium and dynamic) needed to get the driving force correct?

3) Page 29, Lines 16-20: How can the mass of layers stay constant if the layers are absorbing mass from the gas phase or releasing mass to the gas phase? I think a cartoon would help a lot here as well, but I leave it to eh authors’ discretion. It’s difficult to understand how material can be transferred between layers instantaneously due to numerical inconsistencies and yet fidelity with respect to internal gradients can still be maintained.

4) Does the ‘explicit’ case make the same assumptions about equilibrium between the internal layers and the gas phase that the ‘implicit’ case does? Is the major feature of explicit-ness the fact that there are 100 layers instead of 4 or 5? If so, are there important differences between this explicit case and another model like KM-GAP? Specifically, how are the fluxes in Eq. 85 calculated? I recommend moving the explanation of the explicit model to the methods section as well.

### **Technical Issues:**

Page 2, Line 25-26: Can the authors add a quantitative measure here of what good agreement means?

Page 3, Line 12: Please consider rephrasing “species need to be lumped” to “it can be advantageous to lump species”

Page 4, Line 26: What minimum solubility is implied by a species that completely dissolved in the aqueous phase at  $0.01 \mu\text{g m}^{-3}$  of water? My guess is one with a solubility of  $1 \times 10^{-4} \mu\text{g m}^{-3}$ ? Please state this somewhere.

Page 9. Lines 9-10: The authors should state why they bother using parameters from UNIFAC at all, instead of just using parameters from AIOMFAC. The text reads as if AIOMFAC can give all the parameters, but the authors have chosen to use both methods. This could be a point of inconsistency.

Page 31, Line 8: “...concentration and of organic particulate-phase...”

Page 34, Lines 16-20: Can't see this from figure 4.

Figure 4: It is difficult to see most of the action in these plots. It does not seem like the low vicinity of the x-axis ( $10^{-12}$  to  $10^{-5}$ ) is necessary. Please consider zooming in.

Section 3.2: Should be moved to before the results discussion.

**Typos:**

Page 3, Line 19: "strongly impact *predicted* OA formation."

Page 3, Lines 13-16: Perhaps replace "the surrogate based methodology" with "surrogate-based methodologies" to emphasize their use throughout the field.

Page 5, Line 24: Please remove the second occurrence of "dynamic". i.e. "In the dynamic approach, the condensation and particle diffusion of organic compounds"

Table 4 Caption: Reverse the last comparison. "...very high for compounds with  $K_p \leq 0.01$ ". The last sentence should read "A and B types are, respectively, hydrophilic..."