

Interactive comment on “Semivolatile POA and parameterized total combustion SOA in CMAQv5.2: impacts on source strength and partitioning” by Benjamin N. Murphy et al.

Anonymous Referee #2

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The manuscript by Murphy et al. reports on the revised treatment of organic aerosol (OA) in the Community Multiscale Air Quality Model (CMAQ) v5.2. The revised treatment of OA includes: 1. partitioning and gas-phase aging of primary OA (POA), and 2. a new model species “pc” (pcVOA, pcSOG, pcSOA) that represents the missing emissions and processes that may be associated with secondary OA (SOA) formation from urban combustion sources. Model simulations are performed at 4- and 12-km resolution and evaluated at different time periods, seasons, and US locations using surface network monitor data. The changes in the model representation of OA generally result in better correlation and improved bias; the average contribution of the new model species, pcSOA, to OA was ~39% in winter and ~24% in summer. The model evalua-

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tion is thorough and may contribute to elucidating the relative importance of emissions vs. processing in specific locations. The manuscript is generally well written and appropriate for publication in ACP. Specific comments and suggestions for revision are provided below.

In the abstract and introduction the authors suggest that given the quality of the model predictions using the “simple” parameterization presented, caution should be exercised when using more complicated parameterizations (higher number of uncertain parameters). I do not see a fundamental difference with the approach presented here and others. SOA formation depends on the amount of precursor, the extent of oxidation, and volatility of the resultant oxidation/reaction products. The approach presented is a hybrid of existing approaches (including VBS for POA) and relies on arguably uncertain parameters for each of the factors controlling SOA from the new precursor (scaling factor for POA to determine pcVOC, reaction rate constant with KOH to obtain pcSOG, and c^* value to convert pcSOG to pcSOA). The net result of all of the current modeling approaches is that relative to the traditional two-product/non-volatile POA approach, they produce more oxidized OA with a temporal and spatial distribution that is more representative of observations. This is not to say that the changes in the model representation aren't warranted or needed; they are. As articulated by the authors, the changes represent the evolving knowledge of OA formation in the atmosphere. However, all of the current approaches face the same limitations regarding uncertainty in model parameters, a consequence of the complexity and likely variability of processes contributing to SOA formation.

The approach presented combines traditional model representation for VOCs, VBS model representation for POA, and a method based on Hodzic and Jimenez to represent missing sources and processes. It would be useful to see the relative contributions of these processes (by model species) to the total OA predicted. Were any simulations run with only the partitioning and aging of POA or only the consideration of pcSOA? On p. 5, line 34 the authors state that no POA emissions scaling was used to introduce

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SVOCs; however, that is effectively what is done using the pc surrogate species. If combustion source emissions inventories have been revised to reflect the knowledge of dynamic partitioning and missing IVOCs, then these emissions are being double counted by the combined use of a dynamic POA model and the scaling of pcVOC to POA emission rate.

What is the rationale for maintaining the SOA formation pathway for traditional VOC precursors? Isn't this pathway essentially accounted for (or could be accounted for) using the surrogate?

It is recommended that the products of POA evaporation and aging ("OO") be listed in section 2.1, similarly to the directly emitted species, to improve the clarity of Table 1. How are the molecular weights assigned to the "OO" products?

On page 7, line 25 the authors note that no further reactions are considered for pc-SOG/pcSOA, but based on the very low c^* and the rationale for including pcSOA, doesn't the conversion of pcSOG to pcSOA essentially represent these "other" reactions? Given that all of the pc is likely to end up (and stay) in the aerosol phase, it isn't clear what other reactions would be considered or why.

It is suggested that the authors use naming conventions that have been presented previously. For example, "LO-OOA" is presented on pg 9, line 11. Is the same as AMS derived "OOA-II"?

On page 15, line 14: What is meant by wood burning area sources not emitting SOA precursors consistent with pcSOA formation?

The value of c^* for pc is 10^{-3} in the text and 10^{-5} in table 2.

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