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Discussions

Interactive comment on "A naming convention for atmospheric organic aerosol" *by* B. N. Murphy et al.

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Response to Referee #2

General comments:

(RC2.1): The authors present an interesting and comprehensive framework for naming organic aerosols. While their proposed approach is conceptually sound, I find it difficult to understand how it would apply in practice. It is unclear to me how such detailed naming should be applied to a range of field measurements where, as the authors

acknowledge, the classifications generally must be operationally defined. Further, in order to assign all prefixes and suffixes (e.g., ELV, iv, etc.), isn't it necessary to track molecular information for all precursors and reaction products? That level of information is rarely available, unfortunately. It seems unlikely that that level of detail would additionally be tracked in models. For these reasons, I struggle to see how this framework will be broadly applicable in the near future. Though despite my skepticism, the manuscript overall is technically sound, and thus in agreement with the other reviewers, it will be up to the broader scientific community to decide to what extent the proposed naming convention is adopted. The paper is acceptable for publication following the suggested revisions below.

(AC2.1): We thank the reviewer for thoughtful comments on the merits of including the detailed level of information we recommend in the manuscript. We agree with the reviewer that the assignment of all prefixes and suffixes from one study would be a challenging task for a model, and probably infeasible for a field study. However, suitably designed field and laboratory campaigns could make use of varying subsets of these identifiers. We have added examples of such studies to the text (see below). The reviewer also points out an important point echoed by reviewer 1. In order to consistently connect emission (or precursor) volatility to the current OA material being classified, one has to take into account combination reactions (e.g. when SOA-iv and SOA-v react to form one product, what is it called?). We repeat our earlier justification for tolerating this problematic discrepancy though. It is important to communicate properties of organic compounds at the point of emission to the broader community. Source attribution is a major sub-field of research in the air quality community; the problem of defining the line between anthropogenic and biogenic pollution has long been debated in that context, yet the classification continues to resonate because of its usefulness in framing science and policy discussion. The same problem applies to attributing OA to intermediate volatility or semivolatile sources. Knowledge of the contribution of each of these two classes could lead to focused mitigation strategies and thus prove exceedingly beneficial.

Specific comments:

(RC2.2): While extensive hypothetical example names are given in Table 3, the paper would be much improved by including more explicit practical examples to demonstrate exactly how the one should map their laboratory, field, or modeling data/output to the naming scheme. This would particularly help those less familiar with VBS that may not understand how to obtain the necessary C^* values for assigning volatility classes. This appears to be an essential point for readers to grasp, since the volatility labeling is the novel aspect here; without that, the naming scheme essentially falls back to the status quo.

(AC2.2): We have added the following text outlining examples of laboratory, field, and modeling exercises that could benefit from the detailed naming scheme:

“It becomes conceivable, for instance, for a regional-scale modeling study to report the relative contributions to semivolatile OA (SV-OA) by compounds emitted as semivolatile (SV-OA-sv), intermediate volatility (SV-OA-iv), and volatile (SV-OA-v) compounds as a function of season or proximity to major source areas. Although this kind of information has been reported before (Tsimpidi et al., 2009; Murphy et al., 2010; Jathar et al., 2011), imprecise terms like “non-traditional SOA” arose that become much more systematic and clear when the proposed nomenclature is applied.”

“Other useful applications of the proposed scheme come to mind in the context of field and laboratory observations: 1) OA is captured at an observation station and the chemical composition is measured as a function of volatility with the thermal desorption/gas-chromatography/mass-spectrometry (TD-GC-MS). When combined with positive ma-

trix factorization techniques, source attribution combined with knowledge of the volatility distribution could yield a suite of OA classes in need of identification. 2) A series of lab experiments are designed to age several OA precursors of varying carbon number (and thus volatility) in a flow tube. The OA formed in the tube is measured with a thermodenuder and the resulting OA yields measured during the campaign can be organized using both volatility prefixes (that of the OA produced in the chamber) and suffixes (that of the precursor species). 3) The emissions of a power plant plume can be captured in a portable smog chamber and measured with a GC x GC vacuum ultraviolet high-resolution time of flight mass spectrometer to obtain a volatility and polarity distribution. The captured emissions can then be aged inside the chamber and resampled to observe effects on volatility. The chemical composition information would yield valuable insights on the apportionment of primary versus secondary OA and the dependence of this apportionment on initial and final volatility.”

(RC2.3): The discussion should also include measurement techniques other than the AMS. The AMS is certainly the most widely used, but there are other significant instruments applied to measuring organic aerosols (e.g., GC/MS, single-particle mass spectrometry, FTIR). The authors should offer additional examples of how these might be applied under the proposed scheme. Since the authors are attempting to transform how the community as a whole names organic aerosol constituents, such additional examples would go a long way toward achieving that goal.

(AC2.3): We have added mention of GC/MS techniques to the discussion, although they have quite similar connections to the naming framework as have AMS techniques. We have added the following line:

“Observations of organic aerosol volatility have been refined as well through the use of gas chromatography (Isaacman et al., 2011; Presto et al., 2012; May et al., 2013a, b; Chan et al., 2013) and thermodenuder (Hildebrandt et al., 2009; Huffman et al.,

2009) methods. Because of the physical importance of volatility to gas/particle partitioning and the widespread attention volatility has received, it makes sense to anchor a proposed scheme to this property."

We have chosen to omit functional-group information supplied by FTIR results, except in the case that they are used to infer source attribution. In our view, results from FTIR analysis fall into a similar category as O:C information. It is indispensable information for the aerosol scientific community; however, not necessarily essential for communication to broader communities as it stands today. We have added the following discussion of FTIR results:

"One can think of other attributes to accommodate with this scheme: for instance, oxidation state (or O:C ratio) or functional group as detected by Fourier transform infrared spectroscopy (Russell et al., 2011). Although there is a wealth of data and analysis in recent literature showing the importance and usefulness of these properties, volatility is most directly relevant for gas/particle partitioning under typical atmospheric conditions, which is most relevant for predicting condensed-phase concentrations and societal impacts. Oxidation state can be further incorporated into this scheme if future observations warrant (e.g. if a direct connection to negative human health outcomes is shown)."

(RC2.4): I have some issues with the "simplified" naming schemes outlined in section 4: 1. The authors should clarify that at the threshold of 320 μg/m^3 (line 19 of pg 29995) POA compounds have C* values such that effectively all of the compound is in the particle phase (While conceptually obvious, it reads as if any compound that partitions to the particle phase at 320 μg/m^3 is POA.) 2. Again, it is unclear how the non-VBS researchers should determine how to classify their data according to the presented scheme for use in policy decisions. This could create confusion among both scientists and policymakers. 3. The scientific rationale and policy benefit of lumping several

non-traditional SOA categories into "POA" are not clear, particularly from semi-volatile precursors.

(AC2.4): We thank the reviewer for useful comments on this section. 1. We have clarified the discussion of the POA/SOA split.

2. We stress here that the naming scheme, although heavily referencing studies based on the volatility basis-set concept, is not dependent on it for use or implementation. VBS and non-VBS researchers alike commonly have some idea as to the volatility of the compounds they are focused on in order to address gas/particle partitioning phenomena, which is our primary focus since it has such direct impacts on mass loading.

3. This point is well-taken. In regards of scientific rationale, we would not expect expert scientific dialogue or reporting to make use of the "simplified" scheme very often. However, the policy benefit of lumping non-traditional SOA categories is also admittedly difficult to determine. It is true on the other hand, that the term non-traditional SOA and its definition (or lack thereof) is very difficult to communicate to non-experts. Our intention with this "simplified" scheme is to alleviate the confusion attached to terms like this in particular, which have meaning in a historical context but not necessarily in an objective scientific or policy context.

We agree that lumping material emitted in the gas phase (as at least some of the semivolatile material should be) with POA is somewhat confusing, but we view this as an unavoidable challenge when grappling with processes as dynamic as gas/particle partitioning and mass transfer. On the opposite side, it is possible for freshly emitted intermediate volatility compounds to be cooled dramatically, if caught in a particularly strong convective updraft for instance, and to condense to the particle phase in the upper atmosphere without reacting. Our solution to these complicated challenges is to standardize the temperature and OA concentration of the division, two properties that we know to be of major influence. Moreover, the temperature and concentration are relevant for most ambient concentrations. Any approach will have difficulties, but we believe this one to be the most consistent and defensible.

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