

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

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Received and published: 6 April 2014

article

**acp-2013-734**

**Response to Referee #3**

**(RC3.0):** It is indeed a daunting and ambitious task to propose a naming convention for organic aerosol and this attempt is one that should be applauded. The convention starts from the useful and pragmatic VBS approach, defining organic particulate material largely in terms of volatility as the major determinant of the phase state of

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the organic material. Again, this is largely appropriate and most of the concepts within our current understanding of organic aerosol seem to fit reasonably well within this context. I am fully in agreement with the need to be much more rigorous and systematic in classifying and describing both the particulate and vapour components in organic aerosols. I am also in agreement that the broad classes of descriptor that are described are also broadly the ones that need to be reported in modelling and measurement studies; it is in the exact terminology that I have problems. In agreement with the other review, I feel that time will provide the most challenging test of the proposed convention. Only if it is comprehensively capable of encompassing current and emerging understanding of this complex area should its adoption be encouraged and persistence be guaranteed. Before publication, I would like to solicit responses from the authors on the following points:

**(AC3.0):** We thank the reviewer for his critique, and share his assessment of the need for a convention and the essential capabilities that one must have to be successful.

**(RC3.1):** p29990: I am unsure of the reasoning behind use of the alphabetic volatility descriptors. They appear rather arbitrary and relative. The basis set has already clearly defined the decadal bins of saturation concentration at 298K which are objective and absolute and hence not open to interpretation - there is no need to try to impose new strict boundaries here to what is subjective terminology. I have been uncomfortable for some time with the quite arbitrary low volatility cutoff of the SVOC class definition, where historically any particle component that non-negligibly equilibrates with the vapour phase might be considered "semi-volatile". I foresee the same sort of problem here as has occurred with the terminology ultrafine, where UFPs have been defined as particles less than 3 nm, 10 nm, 50 nm or 100 nm in various recent publications to my definite knowledge, with probably very many more. Indeed, this is already happening (see the sentence starting line 18 on p29993). For these

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reasons, I am not convinced by the sentence starting on line 25 on p29991 "In general, the framework allows the communication of available information about volatility and source while avoiding confusing and possibly contradicting terminology". It would be more convincing if numeric saturation concentration descriptors were used in the prefix and suffix. For example a prefix or suffix of "1,2" meaning a component between 10 and 100  $\mu\text{g m}^{-3}$  or of "1.5" referring to a classification of saturation concentration 32  $\mu\text{g m}^{-3}$ . A cynical rephrasing of the statement in line 23 of p29993 might be "uses the quantitative effective saturation concentration to distinguish between classes, and replaces them with qualitative, subjective descriptors with artificial strict definitions".

**(AC3.1):** As stated in our responses to reviewer 1 (AC1.1 and AC1.3), the motivation behind the alphabetic classes derives from our intention to introduce a naming convention that effectively bridges the expert aerosol research community with the broader scientific and policy communities, while remaining useful and precise within the expert community itself. We think that alphabetic groups go a long way to reducing the barrier to understanding that non-experts have when engaging with the complexities of current organic aerosol science. Numeric prefixes or suffixes, on the other hand, may be easier to confuse and harder to keep track of for those not intimately familiar with the concepts of volatility, saturation concentration, and even logarithms.

The low volatility cutoff is an interesting concern; we have defined the range of  $C^*$  for semivolatile behavior to span the range of ambient OA concentrations. Thus ours is slightly stricter than the reviewer's. However, "low volatility" does not necessarily need to imply "no vapor phase". The material in the low volatility range we have defined will actually be non-negligibly accessible to gas-phase aging at relevant atmospheric oxidant levels. We have added the following text discussing these important points to the manuscript:

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Section 2, Paragraph 6: "The mapping of each of the semi-quantitative volatility classes to quantitative measures in  $C^*$  space has been carefully considered. Semivolatile material (SV;  $0.32 \mu\text{g m}^{-3} < C^* < 320 \mu\text{g m}^{-3}$ ) partitions significantly to both condensed and vapor phases at OA concentrations relevant for the troposphere. Extremely low volatility (ELV) material on the other hand, has such low vapor phase levels that it is essentially inaccessible to gas-phase oxidation and experiences no appreciable aging via this route during its atmospheric lifetime. At the other end of the spectrum, volatile material with  $C^* > 3.2 \times 10^6 \mu\text{g m}^{-3}$  is consistent with the legacy acronym, volatile organic compound (VOC) and does not partition at all to the aerosol phase in the atmosphere."

**(RC3.2):** p29990: I have several problems with the second letter in the source root name: i) M representing mass could easily be confused with matter or material in other literature (particularly that concerned with air quality and policy). Indeed, use of OM to represent organic mass (in contrast to OA or OG) appears to erroneously imply that OA or OG do not have mass based units. ii) since an aerosol comprises the entire suspension of particles in the carrier gas, OC for condensed organic or OP for particulate organic would appear to be preferable to OA (though the former would then be inevitably confused with organic carbon of either phase and the P in the latter could be confused with primary). This is actually at the root of a problem with the interpretation of primary emission ageing, where the primary components that are oxidised prior to condensation could either be the gaseous components in the original primary organic aerosol (using its conventional definition to mean gaseous plus particulate components) or evaporated condensed components. The failure to adopt this definition of aerosol to include all phases is an extremely widespread source of error and confusion and it is extremely important that "aerosol" is not used to mean only the condensed material in the aerosol. iii) OG is probably not as precise as OV, since vapour is a condensable gas (i.e. at a T lower than its critical point). Since we are concerned with the organics in the aerosol that can partition, it might be

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considered useful to separate the non-condensed organics into those that will always remain as "carrier gases" and those that could condense with changing T, RH and P under conceivable atmospheric conditions. iv) OM has previously been widely used to denote only the particulate organic mass (to contrast with the particulate mass of organic carbon, OC) rather than the total organic mass in both phases. I don't have any clever suggestion to resolve these problems, but would probably resort to subscripting this second letter, using for example POMT, SOMV and SOCP to mean Total Primary Organic Material, Vapour Phase Secondary Organic Material, Particulate Phase Secondary Organic Carbon etc...

**(AC3.2):** We have incorporated the reviewer's comments (along with reviewer 1) and revised the treatment of organic carbon and phase in the scheme. This revision avoids most of the difficulties the reviewer points out.: i) we have instead adopted a subscript for identifying the phase of organic matter or organic carbon. ii) we have decided not to overturn the commonly held misconception of the definition of aerosol in this scheme. As previously stated, an overarching concern is comprehension by the policy community, which already adapted to the widespread equality between "particle" and "aerosol". It is quite possible that redefining that basic element would cause much more confusion than clarity. Instead we explicitly recommend that OA be synonymous with OAp (or OAparticle) and that other phases be identified similarly (e.g. OAvapor, OAtotal). The basic terms OA, POA and SOA would then remain unaltered. iii) we agree to the preferential use of "vapor," especially considering the current focus on issues relating to "glassy" organic particles. iv) we have adopted the subscript in our revised scheme.

**(RC3.3):** p29991, line 3: The absence of the "P" or "S" indicator meaning that the classification is "both" primary and secondary could present difficulties. It could instead be that it is unspecified or unknown, which could well be the case unless the

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classification is only generated by a model. p29991: Similarly difficult is the lumping of the "aq" pathway modifier alongside the "a" and "b" source modifiers. Surely both "a" and "b" can also be "aq" in origin, for example. Theoretically, there is also no reason why some biomass burning derived VOCs could not be oxidised to produce "aq" particulate. Similarly, surely all "c" particulate is also "a" (likewise all "m" being a subset of "b"). Whilst all the modifiers are useful, I don't think their meanings are quite comparable in what they are classifying. Also, the meaning of the absence of modifiers is not defined - is it that the origin is unknown or that it is not of the origin of the absent modifier.

**(AC3.3):** We have addressed the issues related to source attribution in our responses to reviewers 1 and 2 (AC1.4, AC2.1). We are not sure about the reviewer's distinction between compounds that are "both" primary and secondary and ones that have "unknown" or "unspecified" origin. In our view, if the classification is not given, then the material should be assumed to comprise of unknown contributions from both types. The same philosophy applies to the omission of other identifiers. We agree that the meanings of the different modifiers are not always comparable and that some are subsets of others. This does not interfere with their function of specifying with greater detail OA that is otherwise of less known origin.

**(RC3.4):** p29993: I am not sure I understand the statement starting on line 27, where the naming convention allows for operationally-defined measurement nomenclature in the source root term. The convention seems to lose some of its unifying capability by allowing these more imprecise terms to replace the source type. I am not fully convinced that the community will not continue to use their own favourite nomenclature for particular OA specialisms, particularly in field studies, routinely dropping the suffix and seldom providing measurements able to define the prefix. However, there may be a perfectly reasonable argument for allowing this which I have missed. Is it simply to

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recommend a formalism to allow the prefix (and suffix) to be added?

**(AC3.4):** The reviewer is correct that part of the intention here is to solidify a formalism for the suffix and prefix to be added to other descriptive names for organic compounds currently in use. Meanwhile as the field evolves and other properties are explored (e.g. oxidation state, functionality, polarity) this formalism will hopefully provide the skeleton into which developed nomenclature can be assembled, while preserving the important distinctions we are proposing here.

**(RC3.5):** p2994: I particularly like section 4, which pragmatically identifies the need to map the proposed convention onto the traditional POA/SOA model and the recommended approach is promising. The caveat in the last sentence of section 4 is also appropriately strong!

**(AC3.5):** We appreciate the reviewer's feedback here.

**(RC3.6):** Along with the other reviewer, I am also curious about why the authors have chosen to omit explicit reference to the elements of the 2-D basis set encompassing the O:C ratio or oxidation state space, which allows further description of aerosol properties in terms of increasingly measurable / predictable quantities. I think a naming convention that used numerical prefixes and suffixes representing the coordinates on the 2-D VBS and a source root name that was a little more precise and consistent (e.g. 1,2,0.6- POMP -2,3,0.4 representing mass of primary particulate organic material currently in C\* bin 10-100  $\mu\text{g m}^{-3}$  and of O:C ratio 0.6 but emitted in bin 100-1000  $\mu\text{g m}^{-3}$  with O:C ratio of 0.4) would make a valuable and probably more future proof contribution.

**(AC3.6):** Here we again refer to our responses to the first reviewer (AC1.1;AC1.2).

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**(RC3.7):** Throughout the manuscript, it is not completely clear what is being classified. Is it envisaged that the convention is to be applied to aerosol bulk mass, a particular fraction of the mass, individual particles of variable mixing states or specific components within either individual particles or ensembles of particles? Real air parcels may contain, for example, some particles with secondary components of biogenic origin condensed on anthropogenic mixed BC/OC combustion particles in an ensemble that also contains particles that have been long-range transported across the marine environment from biomass burning regions. The classification of bulk samples in terms of the convention would become very unwieldy if it were to consider all of the sources and properties in an ensemble, but will lose history and mixing state information if it is used to specify a mass weighted average value. More importantly - how do you calculate the mass weighted average of a non-numerical descriptor? The authors should include a discussion of the possible uses and applications of the convention and what information would be preserved and lost in various example cases.

**(AC3.7):** The most common application of this convention likely would be to bulk mass or mole contributions as it is in current studies. The connections between this perspective and that of mixing states within individual particles or among ensembles of particles is directly analogous to well-trodden applications involving familiar aerosol components as the reviewer points out. We would not expect one study or figure to report bulk sample composition as a breakdown of all of the possible classifications at once. Instead, any study would have to lump species appropriately in order to maximize both meaningfulness and clarity. As the reviewer has acknowledged, the usefulness of the proposed framework in this endeavor will remain to be seen. While mass-weighted averages are valuable, the reviewer is correct that the underlying volatility distribution will be necessary to achieve such a result. The lumped alphabetic descriptors are not meant to necessarily fill that need, but to make accessible a ready terminology for de-

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scribing the relative contributions of compounds of broadly varying volatility. We refer the reviewer to our response to reviewer 2 (AC2.2) where we describe a few examples of field and laboratory studies where capabilities of the nomenclature are assets.

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