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# A naming convention for atmospheric organic aerosol

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# Abstract

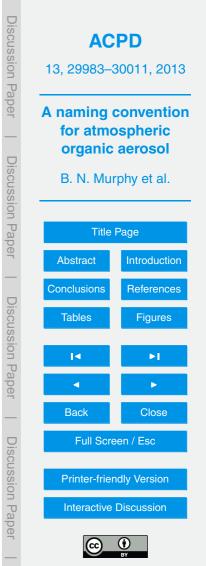
We present a naming convention for classifying organic aerosol (OA) components relevant to laboratory studies, ambient observations and models. The challenge of developing a unified, systematic naming system is formidable, due to the wealth of chemical

- <sup>5</sup> species involved in atmospheric OA, the distribution of these species between multiple simultaneously occurring phases, the large number of possible formation pathways, the growing diversity of measurement techniques available, and the numerous contexts in which OA is discussed. We propose such a system based on the volatility basis set approach that lumps organic compounds by similar effective saturation concentration.
- The volatility classes included in this convention (extremely low volatility, low volatility, semivolatile, intermediate volatility, and volatile), combined with more commonly used terms (e.g. primary and secondary OA, biomass burning OA, etc.) are able to describe and distinguish between several different routes of OA formation in the atmosphere, making them useful for communicating model, laboratory, and field results. Also useful
- is the addition of a suffix representing the volatility of the OA mass or its precursor during emission. This helps connect the current, dynamic view of OA phenomenology with the traditional, static one. Connections between the terms proposed here and observational techniques in the field, including dilution sampling, aerosol mass spectrometry, etc., are also discussed.

### 20 1 Introduction

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Atmospheric aerosols consist of both inorganic and organic compounds (Seinfeld and Pandis, 2006). Myriad sources contribute significantly to the organic aerosol (OA) burden, complicating the analysis of OA formation, growth and removal. Wood burning (residential, prescribed outdoor, forest fires, etc.), energy generation, manufacturing, automobile use, solvent use, shipping (by boat, train, or aircraft), cooking, emission of volatile vapors from plants, sea spray, and other activities all contribute to OA formation



at urban, regional, and/or global scales. After emission, these compounds are susceptible to oxidation processes that may significantly alter their structure and properties. For these reasons, defining a succinct, self-consistent naming convention is challenging. Moreover, ambiguity from an insufficient nomenclature can lead to miscommunication

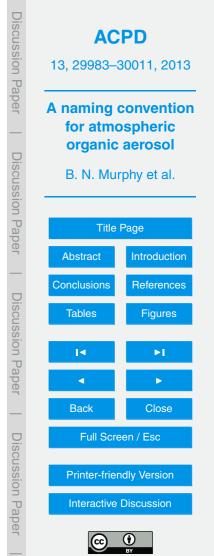
- or confusion of scientific results and conclusions. Because OA formation has important environmental consequences that policy-makers and the general public must address, a viable naming convention should be straightforward and readily understood by non-experts. However, it should also be detailed and flexible to communicate as much information as possible about the origin and chemical nature of OA mass. Before proposing
   such a naming convention, we review past attempts to classify OA over the last two
- decades and the specific challenges that have emerged.

Initially, OA mass was described by just two classifications: primary organic aerosol (POA) and secondary (SOA). POA described presumably non-volatile and inert OA mass emitted in the particle phase from a source, while SOA described material be-

- ginning its atmospheric lifetime as a volatile gas and, after oxidation and condensation, forming condensable (typically semivolatile) organic aerosol (Seinfeld and Pandis, 2006). In this original framework POA and SOA had different sources, volatility and chemical characteristics and this simple categorization was sufficient to describe the then-understood complexity of OA (Pandis et al., 1993). Most chemical transport mod-
- els (CTMs) using this simple framework predicted a majority of the OA in the atmosphere to be POA due to its nonvolatile and nonreactive nature (Chung and Seinfeld, 2002; Gaydos et al., 2007; Karydis et al., 2007).

As new observational techniques (e.g. aerosol mass spectrometry, AMS) emerged, studies like Zhang et al. (2005) found it useful to distinguish between OA mass that

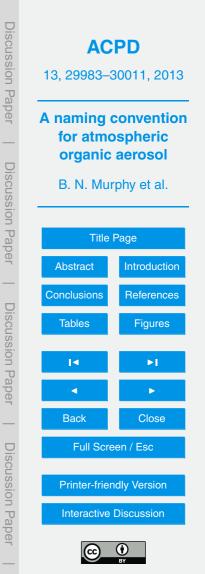
is comprised of highly reduced molecules (hydrocarbon-like OA, HOA) and mass that is consistent with highly oxygenated compounds (oxygenated OA, OOA). Ambient OA was found to contain significantly more OOA than HOA (Zhang et al., 2005; DeCarlo et al., 2010). This view was at odds with what a traditional POA/SOA model would



predict assuming that HOA generally aligns with POA and OOA with SOA (Shrivastava et al., 2008).

Several pieces of evidence emerged to help explain this discrepancy. The traditional model assumed that the effects of oxidation of organics could be accounted for by con-

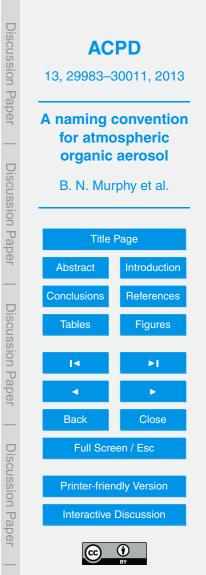
- sidering only the first generation of reactions between organic molecules and atmospheric oxidants (e.g. hydroxyl radical, ozone, and nitrate radical) (Pandis et al., 1993; Griffin et al., 1999; Strader et al., 1999). It is now clear from smog-chamber experiments that semivolatile OA components formed from the oxidation of atmospherically-relevant molecules like xylene (Loza et al., 2012),  $\alpha$ -pinene (Salo et al., 2011; Tritscher et al.,
- <sup>10</sup> 2011; Donahue et al., 2012; Henry et al., 2012), and  $\beta$ -caryophyllene (Alfarra et al., 2012) continue to react with atmospheric oxidants. Whether this continued oxidation leads to a net enhancement or loss of ambient OA mass is unclear due to the number and complexity of interactions that occur.
- A second piece of evidence addressing the disagreement between the traditional <sup>15</sup> conceptual model of POA/SOA and AMS observations of highly oxygenated material was reinforced when Lipsky et al. (2005), Grieshop et al. (2009) and Robinson et al. (2007) argued that POA emissions are substantially semivolatile when diluted to ambient levels. Observations of semivolatile partitioning were not new; Fraser et al. (1997, 1998) measured the concentration of semivolatile species in both the vapor
- and particle phases from ambient samples. The net transfer to the gas phase reduces the influence of hydrocarbon-like, or reduced organic species in the conceptual model. Moreover, these gas-phase species are susceptible to rapid oxidation that can lead to condensation of secondary products back to the particle phase (Presto et al., 2010; Jathar et al., 2012). Communicating the nature of this OA mass in an effective way
- is problematic. This material was originally accounted for as POA mass, but then it underwent a chemical change. Donahue et al. (2009) called this material oxygenated POA (OPOA), a term that identifies both the phase of the material upon emission as well as its chemical history. Both of these pieces of information are useful for scientific applications.



The added complexity associated with treating POA gas/particle partitioning and the effects of SOA and POA multigenerational oxidation led Donahue et al. (2006) to develop the volatility basis set (VBS) framework to organize all of these species into one continuum based on their volatility. In this scheme, organic mass can be assigned to a volatility bin (lumped surrogate of many species with similar volatility) upon emission

- and can then be moved to higher or lower volatility in this space to account for the effects of oxidation. Chemical transport models have implemented this framework and explored the sensitivity of OA mass predictions to uncertainties in volatility of emissions and effects of oxidation (Lane et al., 2008; Hodzic et al., 2010; Murphy and Pandis,
- <sup>10</sup> 2010; Fountoukis et al., 2011; Murphy et al., 2011; Ahmadov et al., 2012; Bergström et al., 2012). When thinking about an OA naming framework, it makes sense to begin with this VBS conceptual model, since it successfully organizes these complex phenomena. There are some additional complexities that must be considered first, though, in order to achieve a naming convention that is useful in both detailed scientific re-<sup>15</sup> search and regulatory implementation.

It is also common practice to classify OA by its sources rather than its properties. Distinguishing between "anthropogenic" and "biogenic" OA, aSOA and bSOA respectively, is a common approach to assess the contribution of humans to atmospheric particles. Biomass burning organic aerosols (BBOA) are emitted by natural forest fires, prescribed burning practices, biofuel use, and residential wood combustion among other sources. BBOA compounds are often classified separately due to the difficulty in assigning them to either anthropogenic or biogenic sources (Simoneit, 2002; Fast et al., 2009). Aqueous-phase SOA (aqSOA) is formed from the dissolution of organics in cloud droplets, followed by reaction in the aqueous phase and finally evaporation of the liquid water. Recent work has shown that even volatile compounds like glyoxal and methylglyoxal can react in the aqueous phase and contribute to this source of organic aerosol (Carlton et al., 2008; Lim et al., 2010; Ervens et al., 2011; Myriokefalitakis et al., 2011) and the SOA products of these processes may be important on



global scales (Liu et al., 2012). These distinctions (aSOA, bSOA, BBOA and aqSOA)

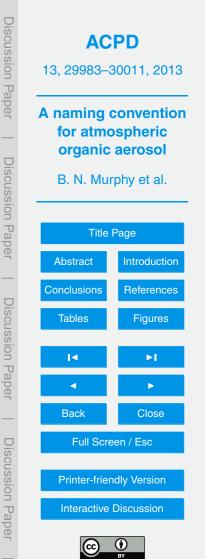
are useful in discussing and reporting model results but are difficult to identify using observational techniques.

In recent years, field observations have led to the emergence of several new classifications for OA. For example, analysis of AMS data has identified the importance of specific sources like cooking OA (cOA), marine OA (mOA), and traffic OA (tOA) (Mohr et al., 2009; Ovadnevaite et al., 2011). Much work has also been accomplished in using <sup>14</sup>C concentrations to attribute OA to fossil (fOA) and non-fossil (nfOA) sources (Lanz et al., 2007; Simpson et al., 2007). The influence of water-soluble organic carbon (WSOC) has been assessed throughout the world with the particle into liquid sampler 10 (PILS) (Sullivan et al., 2004; Hennigan et al., 2009). These classifications are, in gen-

eral, operationally defined by the measurement system used to identify them.

Ambient air quality and emissions standards for OA are based on the traditional POA/SOA conceptual model. For example the US EPA, with regard to organic compounds, has historically required operators of stationary sources to report only emis-

- <sup>15</sup> sions of VOCs and total particulate matter through assessment method 5 (FR, 1971). By encouraging methods 201A and 202 (FR, 2010), the agency acknowledged the importance of capturing both filterable (particulate mass at stack temperature without dilution) and condensable particulate matter (particulate mass at 30°C without dilution), respectively. Unfortunately, these methods are known to have serious positive
- and negative artifacts. Dilution sampling equipment and techniques (Hildemann et al., 1989; Lipsky and Robinson, 2005; England et al., 2007; Li et al., 2011) have been developed over the last 20 yr and are regarded as the most realistic method available for mimicking short-range atmospheric processing (Lee, 2010). Shrivastava et al. (2006), Donahue et al. (2009) and Robinson et al. (2011) argued that measurements should
- <sup>25</sup> be taken at a range of dilution ratios to characterize the volatility distribution of a sample and its likely behavior at ambient conditions. These measurements should include high dilution ratios above 200 : 1 and most importantly on low concentrations similar to ambient conditions. However, the magnitude of necessary dilution depends on the OA mass loading in the emissions plume near the source. The same authors also pointed



out interferences that could exist because partitioning of emissions to the real environment will depend on background OA concentrations. Because of these complications, the line between POA and SOA blurs and careful thought must be put into applying a naming convention to the reporting and enforcement of OA standards in air quality management.

Systematic classifications for organic compounds have been proposed in the past. Donahue et al. (2009) recommended separating species by volatility in line with the VBS framework. Fuzzi et al. (2006) focused instead on distinguishing between 11 sources including biogenic, fossil fuel combustion, open biomass burning, and seaspray among others. That work also acknowledged, though, that classifications by source and those by property should begin to converge as more is learned about OA in general.

We propose an organized and self-consistent naming convention for communicating both OA sources and properties. In Sect. 2, we describe the framework itself, which <sup>15</sup> is fundamentally based on the VBS conceptual model with compounds classified by their volatility. In Sect. 3, we describe extensions to this framework that incorporate the detailed OA classes that have become widely used with increased use of AMS and radiocarbon field observations. Finally in Sect. 4, we show how the proposed framework applies to methods used in air quality management.

### 20 2 Proposed nomenclature

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The proposed classification system describes the properties and sources of atmospheric organic compounds by relying on three components combined in the following syntax:

[current volatility] – [source root name] – [initial volatility]

with the current volatility of the classification indicated by an alphabetical capitalized prefix, the source root name indicated by an acronym currently used in the field, and 29989



(1)

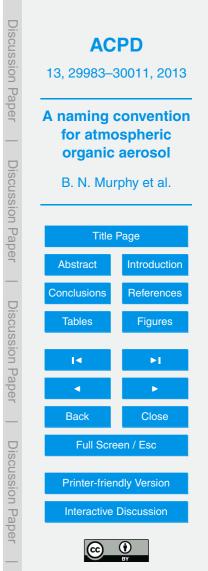
the initial volatility of the species (or its precursor if it is a secondary species) upon emission indicated by a lowercase suffix.

The prefix (Table 1) uses five alphabetical categories to classify organic species by their current volatility (when measured in the lab or field, written to model output, 5 etc.). Extremely low volatility (ELV-), low volatility (LV-), semivolatile (SV-), intermediate volatility (IV-) and volatile (V-) all describe organic compounds along a spectrum of effective saturation concentration at 298 K. Donahue et al. (2006) recommended separating volatility by one order of magnitude in effective saturation concentration, or  $C^*$  (µgm<sup>-3</sup>), and this work follows that framework. The boundaries of each classification have been chosen as the logarithmic average of the representative saturation 10 concentrations (Table 1). For example, the boundary in effective saturation concentration between semivolatile and intermediate volatility OA is  $C^* = 10^{2.5}$  or approximately 320 µg m<sup>-3</sup>. In practice, the definition of effective saturation concentration includes the activity coefficient of each species and so the classification used here may depend on mixing effects. Characterizing these interactions is currently an area of vigorous 15 research, and they may be incorporated into this framework when more thorough understanding has been gained. One approach, similar to the issue of temperature, would

be to define reference compositions to further standardize the classification.

The source root name (Table 2) concisely describes several aspects of the organic species of interest. The core of this nomenclature begins with ("O"), denoting organic, and will be present for every class of compound. Consistent with traditional convention, the species' phase is identified after: aerosol (A), gas (G), or total mass (M). For this scheme, we found it necessary to define OM to indicate the total mass in both the gas and aerosol phases. The total particulate phase organic mass is defined as OA. One

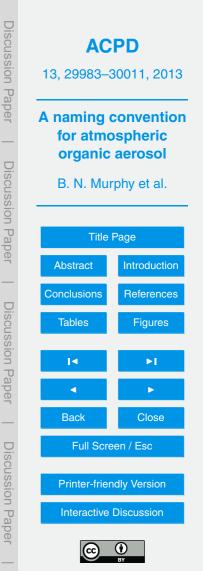
can refer to the mass in any phase due only to carbon by using ("OC") rather than ("O") for the core of the root name. Thus the total particulate-phase organic carbon mass becomes OCA and the ratio of particulate-phase organic mass to organic carbon mass becomes OA/OCA.



The chemical history of each species may be identified via familiar nomenclature as well, with indicators placed before the core ("O"): primary (P), secondary (S), or both (*blank*). Here, we define primary species to be ones that have not undergone any chemical change in the atmosphere, while secondary species have. There is an alternative definition to this distinction, and it is discussed in Sect. 4. The modifiers highlighted in Table 2, which denote source or formation pathway type, have also been in use in the field. Anthropogenic ("a") and biogenic ("b"), biomass burning ("bb") and aqueous-phase ("aq") processes are all subjects of ongoing work and important on local, regional and global scales.

- The optional suffixes presented in the third column of Table 1 identify the original volatility of the species (if it is primary) or its precursor (if it is secondary) upon emission. If the species is primary, then the suffix will necessarily agree in volatility with the alphabetical prefix, since the species has not undergone a chemical change and can be omitted. If either the prefix or suffix is omitted, it is implied that the term identifies
- organic compounds of any volatility. For instance, LV-SOA-iv is mass emitted with intermediate volatility that has reacted to form low-volatility particle-phase mass. Omitting the suffix results in LV-SOA, low-volatility, particle-phase species that have reacted, but their volatility upon emission is not identified. They could have been emitted as lowvolatility particles, intermediate volatility hydrocarbons, or VOCs, etc. Omitting the pre-
- fix from LV-SOA-iv results in SOA-iv, organic mass of any volatility that was emitted with effective saturation concentration in the intermediate volatility range and has reacted. This could describe, for example, the low-volatility products of oxygenated long-chain hydrocarbons and the very volatile fragments of oxidation processes that occurred. Table 3 shows examples of terms under the proposed framework and explanations of their
- <sup>25</sup> contents. The list is not exhaustive though, just illustrative of useful possibilities. In general, the framework allows the communication of available information about volatility and source while avoiding confusing and possibly contradicting terminology.

Connecting this approach to the notation proposed by Donahue et al. (2009) is straight-forward. The definitions of low volatility, semivolatile and intermediate volatil-



ity organic compounds (LVOC, SVOC, and IVOC, respectively) are exactly the same as in that work. The updated scheme proposed here, though, systematically communicates the OA volatility at its source as well. It more directly distinguishes between OPOA (SV-SOA-sv and LV-SOA-sv), non-traditional SOA (SV-SOA-iv and LV-SOA-iv)

<sup>5</sup> and for the first time includes a classification for the low-volatility products of particlephase reactions involving POA (LV-SOA-Iv). It can also be adapted to the large number of specific source categories of OA already mentioned (aSOA, bSOA, bbOA, etc.).

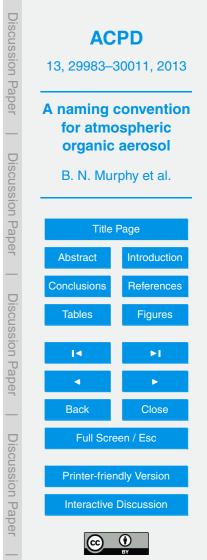
This framework is powerful when applied to developing conceptual models of organic compound evolution in the atmosphere. Although primary organic aerosol emitted in

- the particle phase at low volatility (LV-POA-Iv or LV-POA) can contribute significantly to the total OA burden near sources, it is dwarfed in many regions of the atmosphere by contributions from SOA (Zhang et al., 2007). To understand and predict these contributions, one has to understand the processes that transform compounds with relatively high volatility to ones with volatility low enough to partition significantly to the particle near The nearing compounds is designed to emphasize the import.
- <sup>15</sup> phase. The naming convention proposed here is designed to emphasize the importance of these transformations by identifying a mass' beginning and current volatility.

# 3 Application to laboratory and field measurements

A versatile naming system must accommodate atmospheric and laboratory observations. The proposed framework specifically identifies the current volatility of organic compounds, a property already measured in many field and lab campaigns (Huffman et al., 2009; Lee et al., 2010). As thermodenuder and dilution experiments become more common in the future, it will be critical to report current volatility in a consistent, succinct way.

The root term OOA and other root terms that have been used for classifying observations are presented in Table 4. Under this framework, they can be combined with effective saturation concentration prefixes just like the terms from Table 4, if volatility

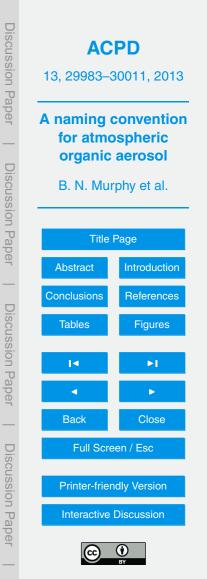


 $OOA \approx SOA = ELV-SOA + LV-SOA + SV-SOA + IV-SOA + V-SOA$ 

since SOA is distinguished from POA here as mass that has been oxidized in the atmosphere. The only exception is that some primary compounds (notably biomass burning emissions) may be partially oxidized during the combustion process. These compounds are technically POA under the proposed framework.

The prefixes LV and SV, identifying low-volatile and semivolatile species, respectively, have already been used extensively to describe two factors that result from positive matrix factorization (PMF) analysis of aerosol mass spectrometer (AMS) data, LV-OOA

- and SV-OOA (oxygenated organic aerosol) (Jimenez et al., 2009; DeCarlo et al., 2010). Because the AMS does not measure volatility, it can only be inferred. The original designations were based in part on the association of LV-OOA with (effectively non volatile) sulfate and SV-OOA with (semivolatile) nitrate, including a tendency to increase with decreasing temperature at night (Lanz et al., 2007). In addition, Jimenez et al. (2009)
- <sup>15</sup> reported the effective saturation concentration of LV-OOA to be at or below 3.2 µg m<sup>-3</sup> and that of SV-OOA to be between 0.01 and 100 µg m<sup>-3</sup>, while thermal denuder measurements have been used to infer the volatility distribution of the OOA factors (Cappa and Jimenez, 2010; Hildebrandt et al., 2010). These estimates generally align with the volatility cutoffs proposed in the current work, but do not strictly agree. As future
- studies yield more information about the volatility of LV- and SV-OOA, possibly through volatility-dependent mass spectra observations, these uncertainties can be reconciled with the strict boundaries proposed here. The same is true for the other root terms. The proposed naming framework uses the quantitative effective saturation concentration to distinguish between classes, not qualitative observations.
- The flexibility of the proposed framework with regard to describing volatility and source type simultaneously will be very useful once measurement techniques are able to report this information routinely. Any type of organic aerosol observed in the field or lab and used in the literature can be incorporated simply by using it as the root



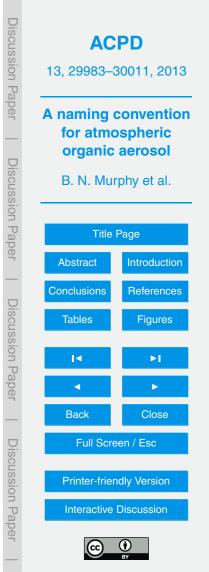
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term. This includes OOA, HOA, WSOC, traffic OA (tOA), fossil-fuel OA (fOA), etc. Lab studies will be able to use the suffix this framework includes, as they will generally be able to identify the volatility of the species at the beginning of an experiment. However, field campaigns will have limited or no access to this information. In these cases, the

- <sup>5</sup> suffix may be omitted and the classification will identify mass with any effective saturation concentration at its source as described in Sect. 2. The treatment of biomass burning OA is a specific example of how the proposed framework can contribute to a more precise description of OA species. BBOA is often classified separately from anthropogenic and biogenic OA in source attribution exercises with the aid of chemical
- tracers (Simoneit et al., 1999; Simoneit, 2002; Abas et al., 2004) or factor analysis of mass spectra (Zhang et al., 2011 and references therein). Although the latter analysis typically assumes that the BBOA factor represents primary OA emissions from biomass burning events, the distinction between primary and secondary often blurs with mixing and chemical processing as pollutants are transported downwind (Aiken et al., 2010;
- DeCarlo et al., 2010). Recent studies have investigated the effects of aging on biomass burning emissions (Cubison et al., 2011; Hennigan et al., 2011; Jolleys et al., 2012). The proposed framework easily distinguishes BBOA between particulate mass from primary emissions (bbPOA) and particulate mass formed through secondary processing (bbSOA). Moreover, phase and volatility information can be incorporated if this information is known. When characterizing source contributions or chemical interac-
- tions (e.g. with NO<sub>x</sub>), one can envision the utility of differentiating low volatility primary biomass burning OA (LV-bbPOA) from semivolatile secondary OA emitted as intermediate volatility species (SV-bbSOA-iv).

# 4 Application to source measurement and policy

Organic aerosol model, field and lab results are synthesized and used to inform policy decisions. Although specific, effective communication within the scientific community is vital, it is likewise important to address the larger community of people interested in air

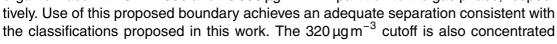


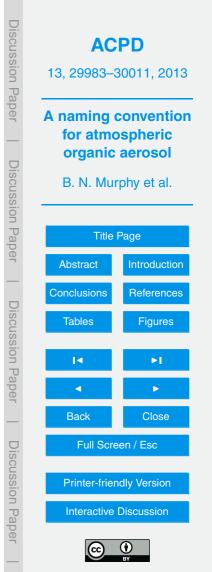
quality, but not necessarily engaged in its detailed scientific issues. One option to bridge this gap would be to recommend a simplified nomenclature, replacing the POA/SOA paradigm while more precisely representing the conceptual model currently adopted by the scientific community. But because the traditional POA/SOA model has such
 a long history and, in general, adequately emphasizes the importance of atmospheric

reactivity, partitioning, and aging that are important for the OA problem, we opt instead to translate our proposed naming convention to the traditional framework and propose standardized definitions to make the connections unambiguous.

Low-volatility emissions may be controlled with technologies targeting particle-phase capture and are well-described as primary OA. At the other end of the spectrum, many VOCs are clearly precursors for secondary OA. Intermediate volatility and semivolatile species may partition to either the particle or gas-phase depending on the temperature and OA concentration of their surroundings. Therefore, in the absence of detailed measurements of the volatility distribution at emission, we propose to standardize the

- <sup>15</sup> conditions at which we distinguish between compounds primarily in the gas and particle phases. Given that in Table 1 we have already distinguished SV-OA from IV-OA with a boundary of saturation concentration ( $C^*$ ) equal to 320 µgm<sup>-3</sup>, we propose defining primary OA as material emitted in the particle phase at an OA concentration ( $C_{OA}$ ) equal to 320 µgm<sup>-3</sup> and T = 298 K. This boundary is somewhat arbitrary but has ad-
- <sup>20</sup> vantages. It preserves consistency between the traditional conceptual model and the detailed framework proposed here. It is high enough in saturation concentration to capture the vast majority of species partitioning to the particle phase at urban and near-source scales. At a  $C_{OA}$  of 320 µg m<sup>-3</sup>, 76 % and 97 % of organic mass with  $C^* = 100$  and 10 µg m<sup>-3</sup> will partition to the particle phase, respectively, according to absorptive partitioning theory (Donahue et al., 2006). On the other hand, 76 % and 97 % of organic mass with  $C^* = 1000$  and 10 000 µg m<sup>-3</sup> will partition to the gas phase, respectively.



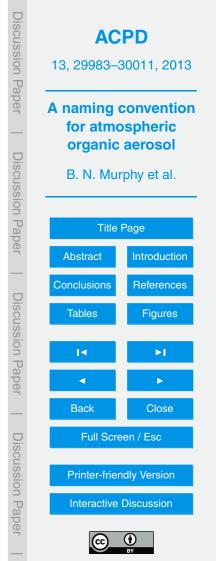


enough to be well-characterized by current dilution sampling techniques that have difficulty with measurements at low, ambient-like, loadings.

The traditional distinction between primary and secondary OA relies on a static definition of primary OA. Under this framework, primary OA has sometimes been classi-<sup>5</sup> fied as the particulate mass emitted from a source and any organic mass enhancement downwind (presumably through oxidation and condensation of organic vapors) has been assigned to secondary OA. Since POA is actually dynamic, three specific pathways to OA formation become difficult to describe:

- 1. Emitted vapor mass condenses to the particle phase, adding mass downwind that
- has not reacted (SV-POA-sv or SV-POA under the proposed detailed framework).
- 2. Emitted particle-phase mass evaporates, reacts and condenses back to the particle phase, changing the chemical nature of the *carbon mass* without changing the loading (SV-SOA-sv under the proposed framework).
- 3. Emitted low-volatlity, particle-phase mass reacts in the particle phase. This mass likely never went through a condensation process but changed the chemical nature of the *carbon mass* without changing the loading (LV-SOA-lv under the proposed framework).

These contradictions have been addressed by standardizing the conditions at which primary OA is defined (above). The traditional paradigm of static primary OA can be represented as the sum of all of the OA terms with suffixes -elv, -lv, and -sv applying to species emitted in the particle phase. OA species emitted at higher volatility (suffixes -iv and -v) are then aligned with secondary OA. Table 5 explicitly maps terms from the detailed framework to the simplified primary/secondary OA model. This mapping applies to the conditions (temperature and OA concentration) outlined above, so there is minimal contribution from intermediate and high volatility organic compounds to primary particles. Thus, the terms IV-POA and V-POA are absent. In short, although this static conceptual model can be a useful representation for the near-source, short



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time scale influence of emissions processes, it is fundamentally flawed and should be avoided in applications requiring physical accuracy.

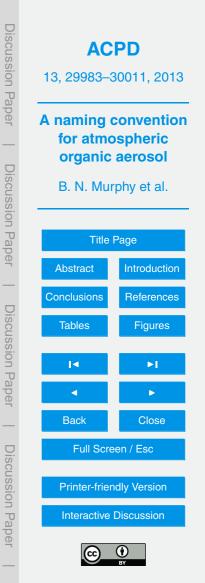
## 5 Conclusions

We have proposed a naming system for classifying atmospheric organic particle and gas compounds. This system is consistent with ongoing field and laboratory studies, and model development. Specifically, it is applicable to the current conceptual model of quite dynamic mechanisms by which these particles form and age. We have chosen to base this system on the volatility basis set, which segregates compounds based on their effective saturation concentration at 298 K. The use of alphabetical prefixes (e.g. ELV-, LV-, SV-, etc.) is standardized in terms of *C*\*. We have also added a lowercase suffix to track the volatility of each species when it was emitted. This suffix can be applied to any *root* term describing the chemical nature of OA (e.g. POA, bbOA, aSOA,

etc.) and bridges the gap between the traditional, static view of the POA/SOA system and the more recent, dynamic view which treats evaporation upon dilution and aging of both primary and secondary material.

Because of the observed semivolatile behavior of POA from many emissions sources, it is important to standardize the conditions at which particles will be defined to be primary. We propose this to be at 298 K and an OA concentration of  $320 \,\mu g \,m^{-3}$ . This concentration is a suitable compromise between the low loadings seen at ambient

- conditions and the higher loadings often encountered when performing source measurements. It also agrees nicely with the proposed division between semivolatile and intermediate volatility OA. In general, this framework provides a standard for communicating detailed volatility, source, and chemical information, and will be useful as the field continues to evolve.
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### References

30

- Abas, M. R., Oros, D. R., and Simoneit. B. R. T.: Biomass burning as the main source of organic aerosol particulate matter in Malaysia during haze episodes, Chemosphere, 55, 1089–1095, doi:10.1016/j.chemosphere.2004.02.002, 2004.
- <sup>5</sup> Ahmadov, R., McKeen, S. A., Robinson, A. L., Bahreini, R., Middlebrook, A. M., de Gouw, J. A., Meagher, J., Hsie, E. Y., Edgerton, E., Shaw, S., and Trainer, M.: A volatility basis set model for summertime secondary organic aerosols over the eastern United States in 2006, J. Geophys. Res., 117, D06301, doi:10.1029/2011jd016831, 2012.

 Aiken, A. C., de Foy, B., Wiedinmyer, C., DeCarlo, P. F., Ulbrich, I. M., Wehrli, M. N., Szidat, S., Prevot, A. S. H., Noda, J., Wacker, L., Volkamer, R., Fortner, E., Wang, J., Laskin, A., Shutthanandan, V., Zheng, J., Zhang, R., Paredes-Miranda, G., Arnott, W. P., Molina, L. T., Sosa, G., Querol, X., and Jimenez, J. L.: Mexico city aerosol analysis during MILAGRO using high resolution aerosol mass spectrometry at the urban supersite (T0) – Part 2: Analysis of the biomass burning contribution and the non-fossil carbon fraction, Atmos. Chem. Phys.,

10, 5315–5341, doi:10.5194/acp-10-5315-2010, 2010.

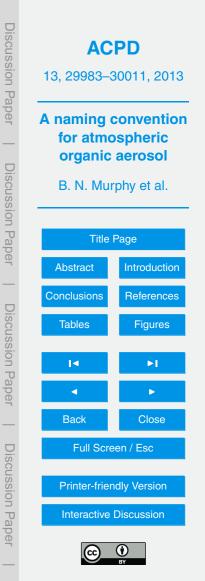
Alfarra, M. R., Hamilton, J. F., Wyche, K. P., Good, N., Ward, M. W., Carr, T., Barley, M. H., Monks, P. S., Jenkin, M. E., Lewis, A. C., and McFiggans, G. B.: The effect of photochemical ageing and initial precursor concentration on the composition and hygroscopic properties of *β*-caryophyllene secondary organic aerosol, Atmos. Chem. Phys., 12, 6417–6436, doi:10.5194/acp-12-6417-2012, 2012.

Bergström, R., Denier van der Gon, H. A. C., Prévôt, A. S. H., Yttri, K. E., and Simpson, D.: Modelling of organic aerosols over Europe (2002–2007) using a volatility basis set (VBS) framework: application of different assumptions regarding the formation of secondary organic aerosol, Atmos. Chem. Phys., 12, 8499–8527, doi:10.5194/acp-12-8499-2012, 2012.

<sup>25</sup> Cappa, C. D. and Jimenez, J. L.: Quantitative estimates of the volatility of ambient organic aerosol, Atmos. Chem. Phys., 10, 5409–5424, doi:10.5194/acp-10-5409-2010, 2010. Carlton, A. G., Turpin, B. J., Altieri, K. E., Seitzinger, S. P., Mathur, R., Roselle, S. J., and

Weber, R. J.: CMAQ model performance enhanced when in-cloud secondary organic aerosol is included: comparisons of organic carbon predictions with measurements, Environ. Sci. Technol., 42, 8798–8802, doi:10.1021/Es801192n, 2008.

Chung, S. H. and Seinfeld, J. H.: Global distribution and climate forcing of carbonaceous aerosols, J. Geophys. Res., 107, 4407, doi:10.1029/2001jd001397, 2002.



- Cubison, M. J., Ortega, A. M., Hayes, P. L., Farmer, D. K., Day, D., Lechner, M. J., Brune, W. H., Apel, E., Diskin, G. S., Fisher, J. A., Fuelberg, H. E., Hecobian, A., Knapp, D. J., Mikoviny, T., Riemer, D., Sachse, G. W., Sessions, W., Weber, R. J., Weinheimer, A. J., Wisthaler, A., and Jimenez, J. L.: Effects of aging on organic aerosol from open biomass burning smoke in aircraft and laboratory studies. Atmos. Chem. Phys. 11, 12049–12064. doi:10.5194/acp-11-
- s aircraft and laboratory studies, Atmos. Chem. Phys., 11, 12049–12064, doi:10.5194/acp-11-12049-2011, 2011.

DeCarlo, P. F., Ulbrich, I. M., Crounse, J., de Foy, B., Dunlea, E. J., Aiken, A. C., Knapp, D., Weinheimer, A. J., Campos, T., Wennberg, P. O., and Jimenez, J. L.: Investigation of the sources and processing of organic aerosol over the Central Mexican Plateau from aircraft measurements during MILACEO. Atmass. Chem. Phys. 10, 5257–5280, doi:10.5104/apr.

<sup>10</sup> measurements during MILAGRO, Atmos. Chem. Phys., 10, 5257–5280, doi:10.5194/acp-10-5257-2010, 2010.

Donahue, N. M., Robinson, A. L., Stanier, C. O., and Pandis, S. N.: Coupled partitioning, dilution, and chemical aging of semivolatile organics, Environ. Sci. Technol., 40, 2635–2643, doi:10.1021/Es052297c, 2006.

- <sup>15</sup> Donahue, N. M., Robinson, A. L., and Pandis, S. N.: Atmospheric organic particulate matter: from smoke to secondary organic aerosol, Atmos. Environ., 43, 94–106, doi:10.1016/j.atmosenv.2008.09.055, 2009.
  - England, G. C., Watson, J. G., Chow, J. C., Zielinska, B., Chang, M. C. O., Loos, K. R., and Hidy, G. M.: Dilution-based emissions sampling from stationary sources: Part 1 Compact sampler methodology and performance, J. Air Waste Manage., 57, 65–78, 2007.

20

- Ervens, B., Turpin, B. J., and Weber, R. J.: Secondary organic aerosol formation in cloud droplets and aqueous particles (aqSOA): a review of laboratory, field and model studies, Atmos. Chem. Phys., 11, 11069–11102, doi:10.5194/acp-11-11069-2011, 2011.
- Fast, J., Aiken, A. C., Allan, J., Alexander, L., Campos, T., Canagaratna, M. R., Chapman, E.,
  DeCarlo, P. F., de Foy, B., Gaffney, J., de Gouw, J., Doran, J. C., Emmons, L., Hodzic, A.,
  Herndon, S. C., Huey, G., Jayne, J. T., Jimenez, J. L., Kleinman, L., Kuster, W., Marley, N.,
  Russell, L., Ochoa, C., Onasch, T. B., Pekour, M., Song, C., Ulbrich, I. M., Warneke, C.,
  Welsh-Bon, D., Wiedinmyer, C., Worsnop, D. R., Yu, X.-Y., and Zaveri, R.: Evaluating simulated primary anthropogenic and biomass burning organic aerosols during MILAGRO: im-
- <sup>30</sup> plications for assessing treatments of secondary organic aerosols, Atmos. Chem. Phys., 9, 6191–6215, doi:10.5194/acp-9-6191-2009, 2009.
  - Fountoukis, C., Racherla, P. N., Denier van der Gon, H. A. C., Polymeneas, P., Charalampidis, P. E., Pilinis, C., Wiedensohler, A., Dall'Osto, M., O'Dowd, C., and Pandis, S. N.:



Evaluation of a three-dimensional chemical transport model (PMCAMx) in the European domain during the EUCAARI May 2008 campaign, Atmos. Chem. Phys., 11, 10331–10347, doi:10.5194/acp-11-10331-2011, 2011.

FR: US EPA Method 5, 40 Fed. Regist. 60, Appendix A, 1971.

25

<sup>5</sup> FR: US EPA Methods 201a and 202, Fed. Regist. 75, 244, 79947 pp., 2010. Fraser, M. P., Cass, G. R., Simoneit, B. R. T., and Rasmussen, R. A.: Air quality model evaluation data for organics, 4: C2–C36 non-aromatic hydrocarbons, Environ. Sci. Technol., 31, 2356–2367, doi:10.1021/es960980g, 1997.

Fraser, M. P., Cass, G. R., Simoneit, B. R. T., and Rasmussen, R. A.: Air quality model eval-

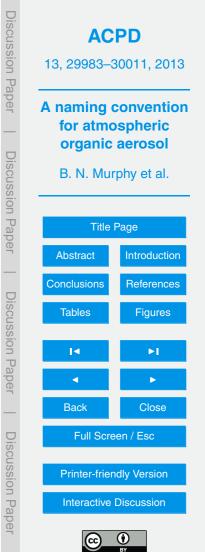
- <sup>10</sup> uation data for organics, 5: C6–C22 nonpolar and semipolar aromatic compounds, Environ. Sci. Technol., 32, 1760–1770, doi:10.1021/es970349v, 1998.
  - Fuzzi, S., Andreae, M. O., Huebert, B. J., Kulmala, M., Bond, T. C., Boy, M., Doherty, S. J., Guenther, A., Kanakidou, M., Kawamura, K., Kerminen, V.-M., Lohmann, U., Russell, L. M., and Pöschl, U.: Critical assessment of the current state of scientific knowledge, terminology,
- and research needs concerning the role of organic aerosols in the atmosphere, climate, and global change, Atmos. Chem. Phys., 6, 2017–2038, doi:10.5194/acp-6-2017-2006, 2006.
   Gaydos, T. M., Pinder, R., Koo, B., Fahey, K. M., Yarwood, G., and Pandis, S. N.: Development and application of a three-dimensional aerosol chemical transport model, PMCAMx, Atmos. Environ., 41, 2594–2611, doi:10.1016/j.atmosenv.2006.11.034, 2007.
- Grieshop, A. P., Logue, J. M., Donahue, N. M., and Robinson, A. L.: Laboratory investigation of photochemical oxidation of organic aerosol from wood fires 1: measurement and simulation of organic aerosol evolution, Atmos. Chem. Phys., 9, 1263–1277, doi:10.5194/acp-9-1263-2009, 2009.

Griffin, R. J., Cocker, D. R., Flagan, R. C., and Seinfeld, J. H.: Organic aerosol formation from the oxidation of biogenic hydrocarbons, J. Geophys. Res. Atmos., 104, 3555–3567, 1999.

Hennigan, C. J., Bergin, M. H., Russell, A. G., Nenes, A., and Weber, R. J.: Gas/particle partitioning of water-soluble organic aerosol in Atlanta, Atmos. Chem. Phys., 9, 3613–3628, doi:10.5194/acp-9-3613-2009, 2009.

Hennigan, C. J., Miracolo, M. A., Engelhart, G. J., May, A. A., Presto, A. A., Lee, T., Sulli-

van, A. P., McMeeking, G. R., Coe, H., Wold, C. E., Hao, W.-M., Gilman, J. B., Kuster, W. C., de Gouw, J., Schichtel, B. A., J. L. Collett Jr., Kreidenweis, S. M., and Robinson, A. L.: Chemical and physical transformations of organic aerosol from the photo-oxidation of open

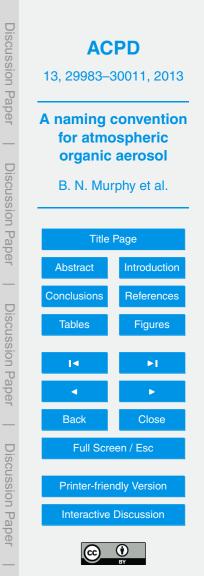


biomass burning emissions in an environmental chamber, Atmos. Chem. Phys., 11, 7669-7686, doi:10.5194/acp-11-7669-2011, 2011.

- Hildebrandt, L., Engelhart, G. J., Mohr, C., Kostenidou, E., Lanz, V. A., Bougiatioti, A., De-Carlo, P. F., Prevot, A. S. H., Baltensperger, U., Mihalopoulos, N., Donahue, N. M., and
- Pandis, S. N.: Aged organic aerosol in the Eastern Mediterranean: the Finokalia Aerosol 5 Measurement Experiment - 2008, Atmos. Chem. Phys., 10, 4167-4186, doi:10.5194/acp-10-4167-2010, 2010.
  - Hildemann, L. M., Cass, G. R., and Markowski, G. R.: A dilution stack sampler for collection of organic aerosol emissions - design, characterization and field-tests, Aerosol Sci. Tech., 10, 193-204, 1989.
- 10
  - Hodzic, A., Jimenez, J. L., Madronich, S., Canagaratna, M. R., DeCarlo, P. F., Kleinman, L., and Fast, J.: Modeling organic aerosols in a megacity: potential contribution of semi-volatile and intermediate volatility primary organic compounds to secondary organic aerosol formation. Atmos. Chem. Phys., 10, 5491-5514, doi:10.5194/acp-10-5491-2010, 2010.
- 15 Huffman, J. A., Docherty, K. S., Aiken, A. C., Cubison, M. J., Ulbrich, I. M., DeCarlo, P. F., Sueper, D., Jayne, J. T., Worsnop, D. R., Ziemann, P. J., and Jimenez, J. L.: Chemicallyresolved aerosol volatility measurements from two megacity field studies, Atmos. Chem. Phys., 9, 7161–7182, doi:10.5194/acp-9-7161-2009, 2009.

Jathar, S. H., Miracolo, M. A., Presto, A. A., Donahue, N. M., Adams, P. J., and Robinson, A. L.:

- Modeling the formation and properties of traditional and non-traditional secondary organic 20 aerosol: problem formulation and application to aircraft exhaust, Atmos. Chem. Phys., 12, 9025-9040, doi:10.5194/acp-12-9025-2012, 2012.
  - Jimenez, J. L., Canagaratna, M. R., Donahue, N. M., Prevot, A. S. H., Zhang, Q., Kroll, J. H., DeCarlo, P. F., Allan, J. D., Coe, H., Ng, N. L., Aiken, A. C., Docherty, K., Ulbrich, I., Grieshop,
- A. P., Robinson, A. L., Duplissy, J., Smith, J. D., Wilson, K. R., Lanz, V. A., Hueglin, C., Sun, Y. 25 L., Tian, J., Laaksonen, A., Raatikainen, T., Rautiainen, J., Vaattovaara, P., Ehn, M., Kulmala, M., Tomlinson, J. M., Collins, D. R., Cubison, M. J., Dunlea, E., Huffman, J. A., Onasch, T. B., Alfarra, M. R., Williams, P., Bower, K., Kondo, Y., Schneider, J., Drewnick, F., Borrmann, S., Weimer, S., Demerjian, K., Salcedo, D., Cottrell, L., Griffin, R. J., Takami, A., Miyoshi, T., Hatakeyama, S., Shimono, A., Sun, J. Y., Zhang, Y. M., Dzepina, K., Kimmel, J. R., Sueper, 30
  - D., Jayne, J. T., Herndon, S. C., Trimborn, A., Williams, L. R., Wood, E. C., Middlebrook, A. M., Kolb, C. E., Baltensperger, U., and Worsnop, D. R.: Evolution of organic aerosols in the atmosphere, Science, 326, 1525-1529, 2009.



- Jolleys, M. D., Coe., H., McFiggans, G., Capes, G., Allan, J. D., Crosier, J., Williams, P. I., Allen, G., Bower, K. N., Jimenez, J. L., Russell, L. M., Grutter, M., and Baumgardner, D.: Characterizing the aging and biomass burning organic aerosol by use of mixing ratios: a meta-analysis of four regions, Environ. Sci. Technol., 46, 13093–13102, doi:10.1021/es302386v, 2012.
- Karydis, V. A., Tsimpidi, A. P., and Pandis, S. N.: Evaluation of a three-dimensional chemical transport model (PMCAMx) in the eastern United States for all four seasons, J. Geophys. Res.-Atmos., 112, D14211, doi:10.1029/2006jd007890, 2007.

Lane, T. E., Donahue, N. M., and Pandis, S. N.: Simulating secondary organic aerosol formation

- using the volatility basis-set approach in a chemical transport model, Atmos. Environ., 42, 7438–7451, 2008.
  - Lanz, V. A., Alfarra, M. R., Baltensperger, U., Buchmann, B., Hueglin, C., and Prévôt, A. S. H.: Source apportionment of submicron organic aerosols at an urban site by factor analytical modelling of aerosol mass spectra, Atmos. Chem. Phys., 7, 1503–1522, doi:10.5194/acp-7-1503-2007. 2007.

15

20

25

5

- Lee, B. H., Kostenidou, E., Hildebrandt, L., Riipinen, I., Engelhart, G. J., Mohr, C., De-Carlo, P. F., Mihalopoulos, N., Prevot, A. S. H., Baltensperger, U., and Pandis, S. N.: Measurement of the ambient organic aerosol volatility distribution: application during the Finokalia Aerosol Measurement Experiment (FAME-2008), Atmos. Chem. Phys., 10, 12149–12160, doi:10.5194/acp-10-12149-2010, 2010.
- Lee, S. W.: Fine particulate matter measurement and international standardization for air quality and emissions from stationary sources, Fuel, 89, 874–882, 2010.
- Li, X., Wang, S., Duan, L., Hao, J., and Long, Z.: Design of a compact dilution sampler for stationary combustion sources, J. Air. Waste Manage., 61, 1124–1130, doi:10.1080/10473289.2011.604556, 2011.
- Lim, Y. B., Tan, Y., Perri, M. J., Seitzinger, S. P., and Turpin, B. J.: Aqueous chemistry and its role in secondary organic aerosol (SOA) formation, Atmos. Chem. Phys., 10, 10521–10539, doi:10.5194/acp-10-10521-2010, 2010.

Lipsky, E. M. and Robinson, A. L.: Effects of dilution on fine particle mass and partitioning of

30 semivolatile organics in diesel exhaust and wood smoke, Environ. Sci. Technol., 40, 155– 162, doi:10.1021/es050319p, 2005.



- Liu, J., Horowitz, L. W., Fan, S., Carlton, A. G., and Levy II, H.: Global in-cloud production of secondary organic aerosols: implementation of a detailed chemical mechanism in the GFDL atmospheric model AM3, J. Geophys. Res., 117, D15303, doi:10.1029/2012jd017838, 2012.
  Loza, C. L., Chhabra, P. S., Yee, L. D., Craven, J. S., Flagan, R. C., and Seinfeld, J. H.: Chem-
- ical aging of *m*-xylene secondary organic aerosol: laboratory chamber study. Atmos. Chem.

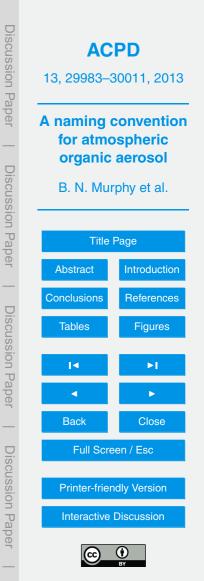
Phys., 12, 151–167, doi:10.5194/acp-12-151-2012, 2012.

Mohr, C., Huffman, J. A., Cubison, M. J., Aiken, A. C., Docherty, K. S., Kimmel, J. R., Ulbrich, I. M., Hannigan, M., and Jimenez, J. L.: Characterization of primary organic aerosol emissions from meat cooking, trash burning, and motor vehicles with high-resolution aerosol

- <sup>10</sup> mass spectrometry and comparison with ambient and chamber observations, Environ. Sci. Technol., 43, 2443–2449, doi:10.1021/Es8011518, 2009.
  - Murphy, B. N. and Pandis, S. N.: Exploring summertime organic aerosol formation in the eastern United States using a regional-scale budget approach and ambient measurements, J. Geophys. Res., 115, D24216, doi:10.1029/2010JD014418, 2010.
- <sup>15</sup> Murphy, B. N., Donahue, N. M., Fountoukis, C., and Pandis, S. N.: Simulating the oxygen content of ambient organic aerosol with the 2D volatility basis set, Atmos. Chem. Phys., 11, 7859–7873, doi:10.5194/acp-11-7859-2011, 2011.
  - Myriokefalitakis, S., Tsigaridis, K., Mihalopoulos, N., Sciare, J., Nenes, A., Kawamura, K., Segers, A., and Kanakidou, M.: In-cloud oxalate formation in the global troposphere: a 3-D
- <sup>20</sup> modeling study, Atmos. Chem. Phys., 11, 5761–5782, doi:10.5194/acp-11-5761-2011, 2011. Ovadnevaite, J., O'Dowd, C., Dall'Osto, M., Ceburnis, D., Worsnop, D. R., and Berresheim, H.: Detecting high contributions of primary organic matter to marine aerosol: a case study, Geophys. Res. Lett., 38, L02807, doi:10.1029/2010gl046083, 2011.

Pandis, S. N., Wexler, A. S., and Seinfeld, J. H.: Secondary organic aerosol formation and trans-

- port: 2. Predicting the ambient secondary organic aerosol-size distribution, Atmos. Environ.,
   27, 2403–2416, 1993.
  - Presto, A. A., Miracolo, M. A., Donahue, N. M., and Robinson, A. L.: Secondary organic aerosol formation from high-NO<sub>x</sub> photo-oxidation of low volatility precursors: *n*-alkanes, Environ. Sci. Technol., 44, 2029–2034, doi:10.1021/Es903712r, 2010.
- Robinson, A. L., Donahue, N. M., Shrivastava, M. K., Weitkamp, E. A., Sage, A. M., Grieshop, A. P., Lane, T. E., Pierce, J. R., and Pandis, S. N.: Rethinking organic aerosols: semivolatile emissions and photochemical aging, Science, 315, 1259–1262, doi:10.1126/science.1133061, 2007.



Robinson, A. L., Grieshop, A. P., Donahue, N. M., and Hunt, S. W.: Updating the conceptual model for fine particle mass emissions from combustion systems, JAWMA, 60, 1204–1222, 2010.

Seinfeld, J. H. and Pandis, S. N.: Atmospheric Chemistry and Physics: From Air Pollution to Climate Change, 2nd edn., John Wiley and Sons, Hoboken, New Jersey, 2006.

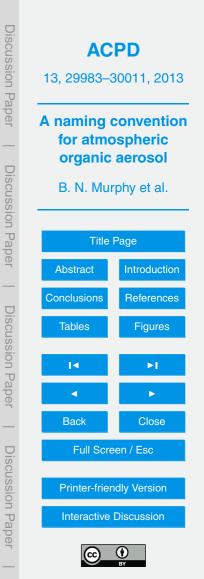
- <sup>5</sup> Climate Change, 2nd edn., John Wiley and Sons, Hoboken, New Jersey, 2006. Shrivastava, M. K., Lipsky, E. M., Stanier, C. O., and Robinson, A. L.: Modeling semivolatile organic aerosol mass emissions from combustion systems, Environ. Sci. Technol., 40, 2671– 2677, doi:10.1021/es0522231, 2006.
- Shrivastava, M. K., Lane, T. E., Donahue, N. M., Pandis, S. N., and Robinson, A. L.: Effects
   of gas particle partitioning and aging of primary emissions on urban and regional organic aerosol concentrations, J. Geophys. Res.-Atmos., 113, D18301 doi:10.1029/2007jd009735, 2008.

Simoneit, B. R. T.: Biomass burning – a review of organic tracers for smoke from incomplete combustion, Appl. Geochem., 17, 129–162, 2002.

- <sup>15</sup> Simoneit, B. R. T., Schauer, J. J., Nolte, C. G., Oros, D. R., Elias, V. O., Fraser, M. P., Rogge, W. F., and Cass, G. R.: Levoglucosan, a tracer for cellulose in biomass burning and atmospheric particles, Atmos. Environ., 33, 173–182, 1999.
  - Simpson, D., Yttri, K. E., Klimont, Z., Kupiainen, K., Caseiro, A., Gelencsér, A., Pio, C., Puxbaum, H., and Legrand, M.: Modeling carbonaceous aerosol over Europe: analy-
- sis of the CARBOSOL and EMEP EC/OC campaigns, J. Geophys. Res., 112, D23S14, doi:10.1029/2006jd008158, 2007.
  - Strader, R., Lurmann, F., and Pandis, S. N.: Evaluation of secondary organic aerosol formation in winter, Atmos. Environ., 33, 4849–4863, 1999.

Sullivan, A. P., Weber, R. J., Clements, A. L., Turner, J. R., Bae, M. S., and Schauer, J. J.: A

- method for on-line measurement of water-soluble organic carbon in ambient aerosol particles: results from an urban site, Geophys. Res. Lett., 31, L13105, doi:10.1029/2004gl019681, 2004.
  - Tritscher, T., Dommen, J., DeCarlo, P. F., Gysel, M., Barmet, P. B., Praplan, A. P., Weingartner, E., Prévôt, A. S. H., Riipinen, I., Donahue, N. M., and Baltensperger, U.: Volatility and
- <sup>30</sup> hygroscopicity of aging secondary organic aerosol in a smog chamber, Atmos. Chem. Phys., 11, 11477–11496, doi:10.5194/acp-11-11477-2011, 2011.



Zhang, Q., Worsnop, D. R., Canagaratna, M. R., and Jimenez, J. L.: Hydrocarbon-like and oxygenated organic aerosols in Pittsburgh: insights into sources and processes of organic aerosols, Atmos. Chem. Phys., 5, 3289–3311, doi:10.5194/acp-5-3289-2005, 2005.

Zhang, Q., Jimenez, J. L., Canagaratna, M. R., Allan, J. D., Coe, H., Ulbrich, I., Alfarra, M. R., Takami, A., Middlebrook, A. M., Sun, Y. L., Dzepina, K., Dunlea, E., Docherty, K., DeCarlo, P.

- Takami, A., Middlebrook, A. M., Sun, Y. L., Dzepina, K., Dunlea, E., Docherty, K., DeCarlo, P. F., Salcedo, D., Onasch, T., Jayne, J. T., Miyoshi, T., Shimono, A., Hatakeyama, S., Takegawa, N., Kondo, Y., Schneider, J., Drewnick, F., Borrmann, S., Weimer, S., Demerjian, K., Williams, P., Bower, K., Bahreini, R., Cottrell, L., Griffin, R. J., Rautiainen, J., Sun, J. Y., Zhang, Y. M., and Worsnop, R.: Ubiquity and dominance of oxygenated species in organic aerosols in anthropogenically-influenced Northern Hemisphere midlatitudes, Geophys. Res. Lett., 34,
- 13801–13806, doi:10.1029/2007GL029979, 2007.

15

Zhang, Q., Jimenez, J. L., Canagaratna, M. R., Ulbrich, I. M., Ng, N. L., Worsnop, D. R., and Sun, Y.: Understanding atmospheric organic aerosols via factor analysis of aerosol mass spectrometry: a review, Anal. Bional. Chem., 401, 3045–3067, doi:10.1007/s00216-011-5355-y, 2011.



| Discussion Pa  | <b>ACPD</b><br>13, 29983–30011, 201 |                     |
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 Table 1. Prefixes and suffixes used for identifying current and emitted volatility, respectively.

| Description              | Prefix | Suffix | Saturation Concentration Bin Center @ 298 K ( $\mu$ g m <sup>-3</sup> ) | Saturation Concentration<br>Range @ 298 K (µg m <sup>-3</sup> ) |
|--------------------------|--------|--------|---|---|
| Extremely Low Volatility | ELV-   | -elv   | ≤ 10 <sup>-4</sup>  | $C^* < 3.2 \times 10^{-4}$                                      |
| Low Volatility           | LV-    | -lv    | 10 <sup>-3</sup> , 10 <sup>-2</sup> , 10 <sup>-1</sup>                  | $3.2 \times 10^{-4} < C^* < 0.32$                               |
| Semivolatile             | SV-    | -sv    | 10 <sup>0</sup> , 10 <sup>1</sup> , 10 <sup>2</sup>                     | 0.32 < <i>C</i> <sup>*</sup> < 320                              |
| Intermediate Volatility  | IV-    | -iv    | 10 <sup>3</sup> , 10 <sup>4</sup> , 10 <sup>5</sup> , 10 <sup>6</sup>   | 320 < <i>C</i> <sup>*</sup> < 3.2 × 10 <sup>6</sup>             |
| Volatile                 | V-     | -v     | $\geq 10^7$   | $3.2 \times 10^6 < C^*$   |

**Table 2.** Examples of root terms for OA classifications.

|            |  | per              | A namina      | convention   |
|------------|--|------------------|---------------|--------------|
| Term       | Description  | ~                |               | ospheric     |
| Modifi     | ers  |                  |               | aerosol      |
| а          | Mass from anthropogenic sources (e.g. aPOA, aSOA, aSOM)  |                  | -             |              |
| b          | Mass from biogenic sources (e.g. bSOA, bPOA, bPOG)   | iscussion Paper  | B. N. Mu      | rphy et al.  |
| bb         | Mass from biomass burning processes (e.g. bbOA, bbPOA, bbSOG)  | SS.              |               |              |
| aq         | Mass from aqueous-phase formation processes (e.g. aqSOA, aqOG)   | ON               |               |              |
| С          | Mass from cooking sources (e.g. cOA)   | Pa               | Title         | Page         |
| m          | Mass from marine or sea-spray sources (e.g. mOA)   | pei              |               |              |
|            |  |                  | Abstract      | Introduction |
| Base       |  |                  | Conclusions   | References   |
| POA        | Primary organic aerosol. This material is emitted in the particle phase and has  |                  | Conclusions   | Ticlerences  |
| DOC        | not undergone a chemical reaction.   | İscı             | Tables        | Figures      |
| POG<br>POM | Primary organic gas. This mass has undergone no reaction in the atmosphere.<br>Total primary organic mass. Sum of POA and POG. | SS               |               |              |
| SOA        | Secondary organic aerosol. This is mass currently in the particle-phase that   | ior              |               | ►I           |
| 30A        | has undergone one or more chemical reactions.  | P                |               |              |
| SOG        | Secondary organic gas. The gas-phase mass produced by at least one chem-   | Discussion Paper |               |              |
| 500        | ical reaction of atmospheric constituent.  |                  |               |              |
| SOM        | Total secondary organic mass. Sum of SOA and SOG.  |                  | Back          | Close        |
| OA         | Total (primary and secondary) particle-phase organic aerosol mass.   | _                |               | een / Esc    |
| OG         | Total (primary and secondary) organic gases.   | Ois              |               | Ben / ESC    |
| OM         | All organic compound mass present in the system in all phases.   | CUS              |               |              |
|            |  | Sic.             | Printer-frier | ndly Version |
|            |  | nF               | Interactive   | Discussion   |
|            |  | Discussion Paper | Interactive   | DISCUSSION   |
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#### Table 3. Examples of organic aerosol classifications under the proposed naming convention.

| Notation                 | Description  | Emissions   |
|--------------------------|--|---|
| ELV-POA-elv              | Extremely low volatility primary organic aerosol emitted with extremely low volatility.  | Extremely low<br>volatility – full<br>partitioning to the                     |
| LV-SOA-elv               | Organic aerosol that is emitted with extremely low volatility and<br>undergoes some chemical change that increases its volatility enough<br>to partition slightly to the gas-phase under certain conditions. | particle phase can be<br>assumed for typical<br>atmospheric conditions.       |
| LV-POA-lv                | Primary organic aerosol existing at low volatility and emitted<br>in the low volatility range. Has not reacted.  | Low volatility –<br>partitions mostly to the<br>particle-phase at             |
| LV-bbOA-lv               | Low-volatility emissions from biomass-burning processes  | atmospheric conditions  |
| SV-POA-sv<br>(or SV-POA) | Semivolatile primary organic aerosol that partitions between the particle and gas phases at atmospherically relevant conditions  | Semivolatile –<br>partitions between<br>particle and gas phases               |
| SV-POG-sv<br>(or SV-POG) | Semivolatile primary organic gas that partitions between the particle<br>and gas phases at atmospherically relevant conditions   | at atmospheric<br>conditions  |
| SV-POM-sv<br>(or SV-POM) | Sum of SV-POA and SV-POG   |   |
| LV-SOA-sv                | Low-volatility, particle-phase products of the multigenerational aging of semivolatile primary organic compounds   |   |
| OA-sv                    | All particle-phase compounds emitted as semivolatile compounds.  |   |
| IV-POG-iv<br>(or IV-POG) | Intermediate-volatility organic gases that have not reacted  | Intermediate volatility –<br>partitions mostly to gas<br>phase at atmospheric |
| SV-SOA-iv                | Semivolatile particle-phase products of the oxidation of intermediate volatility gases   | conditions  |
| LV-SOA-iv                | Low-volatility, particle-phase products of the oxidation of<br>intermediate volatility gases or products of the multi-generational<br>aging of SV-SOA-iv   |   |

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#### Table 3. Continued.

| Notation   | Description   | Emissions                                |
|------------|---|--|
| SV-SOM-iv  | Sum of semivolatile gases and particles from oxidation of intermediate volatility organic compounds   |  |
| OA-iv      | All particle-phase compounds emitted as<br>intermediate-volatility compounds  |  |
| SV-SOA-v   | Semivolatile secondary organic aerosol emitted as volatile gas Volatile – partiti precursors (e.g. toluene, high volatility alkanes, isoprene, $\alpha$ -pinene) almost entirely to the second secon |  |
| LV-SOA-v   | Low-volatility products from the aging of traditional SOA compounds   | phase at atmospheric<br>conditions       |
| SV-SOM-v   | Sum of semivolatile gases and particles from oxidation<br>of volatile organic compounds   |  |
| SV-bSOA-v  | Semivolatile <i>biogenic</i> secondary organic aerosol emitted as volatile gas precursors (e.g. isoprene, $\alpha$ -pinene, terpinene, $\beta$ -caryophyllene)  |  |
| SV-aSOA-v  | Semivolatile <i>anthropogenic</i> secondary organic aerosol emitted as volatile gas precursors (e.g. toluene, high-volatility alkanes and alkenes)  |  |
| LV-aqSOA-v | Particle-phase products of aqueous-phase reactions involving high volatility organic compounds (i.e. glyoxal, methylglyoxal)  |  |
| LV-bbOA-v  | Low volatility products of oxidation of volatile biomass<br>burning emissions   |  |
| LV-POA     | Low-volatility primary organic aerosol  | Unknown volatility at source (e.g. field |
| OA         | Total organic aerosol   | measurement)                             |
| LV-aSOA    | Low-volatility anthropogenic secondary organic aerosol  |  |
| LV-bbOA    | Low-volatility particle-phase compounds from biomass burning  |  |
| SV-bbPOA   | Semivolatile biogenic primary organic aerosol   |  |
| SV-SOA     | Semivolatile SOA  |  |

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Table 4. Organic aerosol classifications used in the literature.

| Notation | Definition   | Proposed Framework  |
|----------|--|---|
| OOA      | Oxygenated organic aerosol   | SOA   |
| LV-OOA   | Low-volatility OOA – $C^* \leq 3.2 \mu \text{g m}^{-3}$            | LV-SOA  |
| SV-OOA   | Semivolatile OOA – $0.01 \le C^* \le 100 \mu\text{g}\text{m}^{-3}$ | SV-SOA  |
| bbOOA    | Biomass burning OOA  | bbSOA   |
| OPOA     | Oxidized primary organic aerosol                                   | ELV-SOA-elv + ELV-SOA-lv+<br>ELV-SOA-sv + LV-SOA-elv+<br>LV-SOA-lv + LV-SOA-sv+<br>SV-SOA-elv + SV-SOA-lv+<br>SV-SOA-sv |

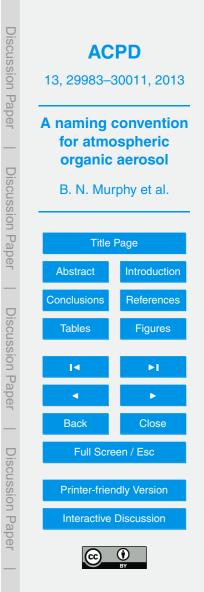


Table 5. Mapping of terms from traditional framework to proposed detailed framework\*.

| Proposed Framework  | Traditional Framework |
|---|-----------------------|
| ELV-POA-elv<br>LV-POA-lv<br>SV-POA-sv<br>ELV-SOA-elv<br>LV-SOA-elv<br>SV-SOA-elv<br>ELV-SOA-lv<br>SV-SOA-lv<br>ELV-SOA-lv<br>ELV-SOA-sv<br>LV-SOA-sv<br>SV-SOA-sv | Primary OA            |
| ELV-SOA-iv<br>LV-SOA-iv<br>SV-SOA-iv<br>ELV-SOA-v<br>LV-SOA-v<br>SV-SOA-v   | Secondary OA          |

\* Boundary between primary and secondary OA is defined at  $C_{\text{OA}} = 320 \,\mu\text{gm}^{-3}$  and  $T = 298 \,\text{K}$ .

