FINAL REPORT

Title: Synthesis of comprehensive emissions measurements and multi-scale modeling for understanding secondary organic aerosol

JFSP PROJECT ID: 14-1-03-44

September 2018

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Abbreviations

BB: biomass burning
BBOP: Burning Observation Project
CTM: chemical transport model
CMAQ: Community Multiscale Air Quality model
EF: emission factor
$PM_{2.5}$: fine particulate matter
GC: one-dimensional gas chromatography
GC×GC-TOFMS: two-dimensional gas chromatography/time-of-flight mass spectrometry
GECKO-A: Generator of Explicit Chemistry and Kinetics of Organics in the Atmosphere
IVOC: intermediate volatility organic compound
I/SVOC: intermediate/semi-volatile organic compound
NEI: National Emissions Inventory
NMOC: non-methane organic carbon
OA: organic aerosol
OP-FTIR: open-path Fourier-transform infrared spectroscopy
PTR-TOFMS: proton-transfer-reaction time-of-flight mass spectrometry
SAPRC: State Air Pollution Research Center gas-phase chemical mechanism model
SOA: secondary organic aerosol
SVOC: semivolatile organic compound
WAS: whole air samples

Keywords

emission factors, intermediate volatility organic compounds, secondary organic aerosol, CMAQ, AIRPACT, wildland fires

Acknowledgements

We thank the organizers and contributors to the 4th Fire Lab at Missoula Experiment (FLAME-IV). We thank the students, postdocs, and faculty that contributed to this work: Isaac Afreh and Lindsay Hatch (UCR team); Chelsea Stockwell (UM team); and Serena Chung, Yunha Lee, and Tsengel Nergui (WSU team). We thank our collaborators S. Kreidenweis and J. Pierce (14-1-03-26), with whom we worked closely on trying to constrain the volatility distributions of gas- and particle-phase organic carbon emissions. We thank Larry Kleinman, Allen Robinson, and Shawn Urbanski for their useful discussions over the years of the project. Finally we acknowledge funding from NASA (Yokelson: NNX14AP45G), NOAA (Barsanti: NA16OAR4310103, NA17OAR4310007) and NSF CAREER (Barsanti: AGS-1753364), as these projects were seeded by the work presented herein and have contributed to our overall understanding, conclusions, and recommendations.

Abstract

The air quality and fire management communities are faced with increasingly difficult decisions regarding critical fire management activities, given the potential contribution of wildland fires to fine particulate matter ($PM_{2.5}$). Unfortunately, in model frameworks used for air quality management, the ability to represent $PM_{2.5}$ from biomass burning (BB) is severely limited. Particularly uncertain is the formation of secondary organic aerosol (SOA). This is due in large part to incomplete identification and quantification of compounds emitted from fires and uncertainties in mechanisms leading to SOA formation under ambient conditions. Thus there is great need for improved emissions inventories and validated smoke models that better capture emissions of intermediate and semi-volatile organic compounds (I/SVOCs) as well as SOA formation and aging as a function of fuel type and burn characteristics. We assembled a uniquely qualified team to: 1) provide improved emission factors (EFs) with an emphasis on those critical to understanding SOA; 2) develop a detailed model to accurately represent SOA in smoke plumes; and 3) use the detailed model as a tool, along with measurements, to implement and deliver an operational modeling framework with an improved ability to predict SOA formation, and thus $PM_{2.5}$, from wildland fires.

We achieved significant improvement in the characterization of gaseous organic compounds, including IVOCs (more abundant than SVOCs), relative to what is currently in the NEI and EPA SPECIATE emissions inventories. Data from four techniques were synthesized into a single EF database that includes over 500 gaseous non-methane organic compounds to provide a comprehensive picture of speciated, gaseous BB emissions. Of the total gaseous EF, 6-11% was associated with IVOCs. These atmospherically relevant compounds historically have been unresolved in BB smoke measurements and therefore are largely missing from emissions inventories. We highlighted some challenges in scaling these laboratory-based EFs to field conditions, particularly given the large diversity of potential SOA precursors and their dependence on fuel type, burn characteristics, and particle loadings. We identified and prioritized a subset of compounds for consideration in air quality models. The identified compounds were screened for published SOA yields; 55-77% of the reactive carbon was associated with compounds for which SOA yields are unknown. Thus we developed reaction mechanisms and SOA parameterizations, needed for air quality modeling, using 0-D box models.

While limited data precluded complete model representation of all compounds, we demonstrated the sensitivity of SOA and $PM_{2.5}$ predictions to newly identified SOA precursors and an increase in total organic carbon. CMAQv.5.0.2 and v.5.2 were used to predict SOA and $PM_{2.5}$ concentrations for August 2013 and 2015. Model results were compared with measurements, including from the Biomass Burning Observation Project (BBOP). $PM_{2.5}$ concentrations were generally underpredicted and relatively insensitive to changes in SOA using CMAQv.5.0.2. However, $PM_{2.5}$ concentrations showed a greater sensitivity to and contribution from BB-derived SOA precursors using CMAQv.5.2. Our BB emissions updates within CMAQv.5.2 generally resulted in a reduction in negative biases in $PM_{2.5}$, and at some sites an overestimation of $PM_{2.5}$. Our integrated measurement-model approach advanced the understanding of key sensitivities and uncertainties for predictions of the contribution of wildland fire emissions to SOA. Future work is needed to: 1) scale laboratory-based EFs of speciated gaseous organic compounds to field conditions (allowing for $PM_{2.5}$ concentration-dependent partitioning); 2) further investigate the chemistry of key new precursors we identified (models and measurements); and 3) better constrain SOA model parameterizations using newly available data.

Project Objectives and Hypothesis

Through the project objectives, we sought to address critical knowledge gaps in: 1) identification and quantification of BB emissions and availability of representative EFs; 2) dominant SOA formation and aging processes in smoke plumes; and 3) the representation of emissions and SOA formation from fires in air quality modeling frameworks. The project objectives and hypotheses were based on questions outlined in Task 3 of the FON: "Contribution of smoke emissions to secondary organic aerosols". A summary update of the objectives and hypotheses follows.

Objective 1: Identify and quantify I/SVOC emissions from selected conifer, shrub, and grass species.

Objective met. We merged all of the EFs measured during the Fourth Fire Lab at Missoula Experiment (FLAME-4) by GC×GC/TOFMS, OP-FTIR, PTR-TOFMS, and 1-D GC/MS into a comprehensive set of EFs for burns of ponderosa pine, black spruce, rice straw, and peat. The total number of identified compounds per fire ranged from 467-569, and the combination of techniques allowed a wider range of compound types to be identified than could be accessed by a single instrument. The resulting publication[1] presents the most comprehensive biomass-burning gas-phase organic emissions inventory to date. Further, 6-11% of the total gaseous non-methane organic carbon (NMOC) EF was associated with IVOCs; these compounds are largely missing from the most widely used emissions inventories, which has implications for predictions of SOA in air quality modeling frameworks.

Objective 2: Quantify SOA formation potentials for I/SVOCs of interest, and identify the most relevant precursors and reaction mechanisms for SOA formation and aging.

Objective met. We identified a large number of compounds within our comprehensive EF database that are likely SOA precursors. All compounds were screened for SOA potential based on their EF, reactivity with OH radical, and carbon number. For all likely SOA precursors, we conducted an extensive literature search for published data on SOA formation (i.e., SOA yields). For many, their SOA yield is either completely unknown or unreported. Of these unstudied (or understudied) compounds, those with the highest SOA potential were identified as top priorities for future studies. Further, for a subset of these prioritized compounds, we estimated the SOA yield using a chemically detailed 0-D box model, and developed model parameterizations.

Objective 3: Evaluate sensitivity of SOA formation to uncertainties in emissions, including as influenced by burn characteristics.

Objective met. Measurement uncertainty, emissions variability, and fuel/MCE dependence were reported Hatch et al. [1] In addition, working with S. Kreidenweis and J. Pierce (JFSP project 14-1-03-26), we investigated how NMOCs (including SOA precursors) are partitioned between the gas and particle phases since higher particle concentrations promotes partitioning to the particle phase. This partitioning has several effects. One practical aspect is that gas-phase EFs measured for I/SVOCs in laboratory settings or near the source in field studies, with high particle concentrations, will be lower than what would be measured in more dilute plumes. More generally, as plumes dilute some particle-phase NMOCs will evaporate to the gas phase depending on their vapor pressure. This reduces the primary OA burden, but adds to the pool of gas-phase SOA precursors. Thus, the relative distribution of NMOC emissions between the gas and particle phase as plumes dilute is needed to model emissions and their chemistry. The gas-particle phase distribution is dynamic and still poorly constrained for some compounds, which is a key uncertainty in modeling emissions and aging.

Objective 4: Modify the AIRPACT framework to include the most relevant SOA precursors and formation and aging mechanisms.

Objective met. Updated speciation profiles for coniferous fuels and crops were developed using the FLAME-IV EFs. These speciation profiles were mapped to lumped model compounds represented in the AIRPACT framework (specifically within the SAPRC gas-phase chemical mechanism and SOA module in CMAQv.5.0.2, and later in CMAQv.5.2). For some of the locations in the CMAQv.5.0.2 modeling domain, maximum predicted SOA increased by a factor of two due to changes in the emissions inventories and speciation profiles for coniferous fuels. CMAQv.5.2 includes an aging mechanism for all combustion-derived SOA (and primary OA), which applies to biomass burning emissions. No other aging mechanisms were considered in AIRPACT. However in CMAQv.5.2, in addition to the updated emissions inventories and speciation profiles, sensitivity runs were conducted in which the total NMOC emissions were increased and the contribution of OC to total $PM_{2.5}$ was increased to better represent recent measurements.[2]

Objective 5: Evaluate implementation of improvements in AIRPACT using satellite products and field data.

Objective met. Model-predicted $PM_{2.5}$ concentrations using CMAQv.5.0.2 within AIRPACT for August 2015 were compared with measurements from air quality monitoring stations in the Pacific Northwest. While maximum SOA concentrations doubled in some locations with the updated emissions inventories, there were no statistically significant differences in $PM_{2.5}$ concentrations and the general negative bias in the model predictions was not improved. One important observation was that the model greatly underpredicted the contribution of SOA (vs. primary OA) to $PM_{2.5}$, in comparison with observations reported by Zhou et al.[1] This is one of the reasons $PM_{2.5}$ in CMAQv.5.0.2 was relatively insensitive to changes in emissions of BB-derived SOA precursors. Predicted $PM_{2.5}$ concentrations using CMAQv.5.2 for August 2013 were compared with measurements obtained during the 2013 BBOP study. The SOA mechanism in CMAQv.5.2 produced a more reasonable SOA (vs. primary OA) contribution to $PM_{2.5}$. When comparing to the air quality network, our updated NMOC EF and speciation profiles led to a general reversal of the negative bias and a positive bias in $PM_{2.5}$ predictions at ~10% of the sites. This may be due to unintended "double counting" of unidentified/unquantified SOA precursors (including evaporated primary OA). Some treatment of this is built into CMAQv.5.2 and may overlap our own model updates.

Objective 6: Identify priorities for future measurement and modeling efforts, including by comparing calculated emission factors with NEI emission factors.

Objective met. We have produced the most comprehensive EF database for speciated, gaseous NMOCs which can be used within a number of air quality modeling frameworks. However, two major limitations exist: 1) uncertainties in scaling laboratory-based EF as a function of fuel type, burn characteristics, and particle loading to effective dilution and fuels implied by model resolution; and 2) absence of reactivity and SOA formation data for newly identified compounds required to constrain model parameterizations. Regarding one, the correlation of gaseous NMOC EFs with fuel type and burn characteristics appears to be relatively robust for laboratory studies.

However, for the wide diversity of NMOCs that we have speciated, this relationship becomes less clear (particularly for more reactive compounds) at the model resolution for which the EFs are applied. For instance, a scaling factor for I/SVOCs that accounts for gas-particle partitioning at the resolution-controlled effective dilution is greatly needed. Thus, one priority, is conducting coordinated measurement efforts (similar to the laboratory campaigns) to produce field-based EFs of speciated NMOCs, which can be compared with laboratory-based values, and to derive volatility distributions of gas- and particle-phase NMOCs. Regarding two, though a large number of potentially important precursors were identified and prioritized for future studies, only a few compounds could be explicitly considered and thus the representation of the newly identified compounds within the AIRPACT modeling framework was limited and poorly constrained. Therefore another priority is the continued pursuit of integrated measurement and modeling studies; in which the future air quality modeling studies will benefit from: 1) the wealth of new measurement data on biomass burning derived precursors and SOA formation (i.e. yields); and 2) the updated model parameterizations and frameworks that are based on the new data.

<u>Hypothesis 1</u>: Improved representation of the diversity of SOA precursors emitted from wildland fires and the processes critical to SOA formation and aging in wildland smoke plumes are needed and can be achieved in current chemical transport models (CTMs).

Partially confirmed. The compilation of gas-phase EFs for speciated organics and our screening procedure confirmed that a number of likely important SOA precursors are not being represented in current air quality modeling frameworks. Further, the quantities of the gas-phase NMOCs, specifically I/SVOCs that are important SOA precursors, may be significantly underestimated in models by using laboratory-based EFs that are not scaled based on total gas- plus particle-phase NMOC. Box model simulations also demonstrated that some of the newly identified compounds were likely to form significant SOA. While these findings improve the our general understanding of the potential for SOA formation from BB emissions, very little data exist on the reaction mechanisms and SOA formation potentials for these newly identified compounds. This lack of data even challenges the use of chemically detailed models, which also rely on such data. Thus, the representation of these diverse precursors in CTMs, while improved, will not be complete or well constrained until further mechanistic data, field validation, and (eventually) parameterizations are available.

<u>Hypothesis 2:</u> Comprehensive analysis of I/SVOC measurements from targeted FLAME-IV studies will allow identification and quantification of important BB-SOA precursors, including their variability as a function of burn and fuel characteristics.

Confirmed. Compilation of data from multiple analytical techniques, applied during FLAME-IV, yielded EFs for a large number of likely SOA precursors, which previously had not been identified and quantified. There were distinct differences in the identities of individual compounds/classes of compounds as a function of fuel type. Subsequent efforts, seeded by the JFSP funding, indicate that the identities and quantities of compounds vary as a function of fuel type and fuel characteristics (e.g., canopy vs. woody fuels vs. duff), which complicates scaling laboratory-based EFs for some compounds/classes of compounds as a function of modified combustion efficiency (MCE). A number of monoterpenes, including camphene, and furan/furan derivatives were identified as likely important for SOA formation.

Hypothesis 3: Multi-scale modeling will allow identification of the mechanisms that describe the bulk of SOA formation in smoke plumes and parameterization for improved representation in CTMs.

Partially confirmed. In CTMs, including CMAQ within AIRPACT, the diversity of NMOCs that serve as SOA precursors are represented by a small number of lumped surrogate products (~5-8). One of the important findings of this work was that not all of the identified compounds could be well represented by the limited number of model surrogates. Developing new reaction mechanisms and SOA parameterizations requires detailed 0-D modeling and/or compilation of measurement data. In the absence of the latter, we were able to develop a gas-phase chemical mechanism for furan/furan derivatives (project leveraged by JFSP) and we also used a 0-D box to derive SOA parameters for a series of monoterpenes, including camphene. CTMs, including CMAQv.5.2, are starting to include upgraded/improved SOA formation mechanisms, but these mechanisms still need considerable refinement and testing.

Hypothesis 4: Laboratory (FLAME-IV) and field (BBOP) data are available to validate advanced BB-SOA representations in model frameworks used by air quality and land managers.

Confirmed. In the first measurement/model comparisons (CMAQv.5.0.2, August 2015), $PM_{2.5}$ predictions were insensitive to changes in predicted SOA (with updated treatment of BB emissions). Comparisons with published data illustrated that likely too much of the total OA in the model was primary, and that with a more reasonable primary to secondary OA distribution, model updates could be better evaluated. The availability of $PM_{2.5}$ concentration data as a function of space and time, with proxy data for the relative distribution of primary vs. secondary OA, were critical for evaluating updates to BB emissions inventories and SOA models.

Background

Wildland fires occur under a variety of conditions and involve a range of plant-based fuels, which vary greatly across global to regional scales. Fires emit high levels of trace gases, including nitrogen oxides (NO_x) and carbon dioxide (CO); I/SVOCs; and primary (directly emitted) PM. During plume evolution, I/SVOCs react to form ozone (O_3) and secondary PM, thereby degrading air quality downwind.[4],[5] BB-PM can additionally influence the radiative balance of the atmosphere directly by scattering or absorbing solar radiation,[6] and indirectly by acting effectively as cloud condensation nuclei.[7, 8] BB is the second largest source of I/SVOCs worldwide. Given the substantial emissions of I/SVOCs, the SOA formation potential from BB is large and may be the second largest source globally, behind emissions from biogenic sources.[9] This large potential for SOA production in smoke plumes is of relevance to the air quality and land management communities in the US, given their desire to minimize potential impacts of wildland fires on downwind communities, as well as on climate, while pursuing effective forest management practices.

BB-PM has been difficult to model effectively in large-scale models used for air quality management (CTMs). First, there is a limitation associated with model inputs. Due to chemical diversity and complexity, identification and quantification of the gaseous organic compounds emitted from fires has been incomplete.[10] In a recent synthesis of laboratory and field measurements, nearly half of the gas-phase species detected could not be identified;[11] demonstrating the need for better characterization of smoke I/SVOCs. Next, there is a limitation in our understanding of the relevant SOA formation and aging mechanisms under ambient conditions, particularly in smoke plumes. This has been discussed widely in the literature.[e.g.,12, 13] Finally, there is the limited representation of SOA precursors and their SOA formation and aging mechanisms in CTMs.[14]

While it is likely that a number of factors can lead to poor simulation of BB-SOA, in this project we focused on three particular limitations: 1) incomplete identification and quantification of gaseous compounds emitted from fires that may serve as SOA precursors; 2) incomplete understanding of the mechanisms that lead to SOA formation in smoke plumes; and 3) over-simplified representation of emissions and processes in current models. Indeed, as articulated in the Smoke Science Plan: The Path Forward,[15] there is a great need for improved emissions inventories and validated smoke models. Emissions inventories need to account for variability in emissions as a function of burn and fuel characteristics. In addition, EFs are needed for all compounds/classes of compounds that can serve as SOA precursors under ambient conditions. In most models, BB-SOA formation proceeds by condensation of surrogates representing the gas-phase oxidation products of a very small number of VOC precursors.[12, 16] Much recent research supports that many previously unconsidered precursors exist,[11, 17-19] and that mechanisms beyond gas/particle partitioning of semi-volatile compounds contribute to ambient SOA formation, including oxidation of lower volatility precursors and aqueous-phase chemistry.[20, 21]

Materials and Methods

Emission Factor Data Compilation and Analysis

This section provides an overview of the procedure for generating the speciated organic carbon gaseous EF database using FLAME-IV data. For a more detailed description see Hatch et al.[1] Calculated EFs using open-path Fourier-transform infrared spectroscopy (OP-FTIR),[22] proton-transfer-reaction time-of-flight mass spectrometry (PTR-TOFMS),[23] two-dimensional gas chromatography/time-of-flight mass spectrometry (GC×GC-TOFMS),[24] and one-dimensional gas chromatography (GC) of whole air samples (WAS) were merged into a single, combined BB emissions database. Overlapping measurements of the same species were counted only once to the best possible extent. Data reduction largely followed the approach described by Yokelson et al. [11] The OP-FTIR data were given precedence because the OP-FTIR is not subject to sampling line artifacts. To combine the PTR-TOFMS measurements with speciated data from the GC techniques, the EFs were compared at each chemical formula, summed over all corresponding isomers measured by the GC×GC-TOFMS and/or WAS instruments. If the PTR-TOFMS EF was more than 2× the integrated GC×GC-TOFMS or WAS EF, both measurements were retained, unless a negative artifact was known to affect the GC data (e.g., cartridge breakthrough), in which case only the PTR-TOFMS measurement was used in the combined EF database. This approach preserves speciated information while retaining the potential for additional unknown emissions unaccounted for by the GC techniques. For cases in which the PTR-TOFMS EF was less than 2× that of the GC×GC-TOFMS or WAS EF, the GC data were used to preserve isomer speciation and the PTR-TOFMS measurement was deleted from the synthesized EF database. However, if only one (predominant) isomer was observed in the GC dataset (e.g., C_6H_6, benzene), the higher EF was used. For isomer groups detected by both GC×GC-TOFMS and WAS, the GC×GC-TOFMS EFs were retained if many more isomers were observed by this technique; if the number of observed isomers was similar at a given molecular formula, the measurement yielding the higher total EF was used in the EF database.

Development of Speciation Profiles

This section describes the process for taking the individual species measured during FLAME-IV and mapping them to model compounds for air quality model simulations. Specific emissions inventories were created for coniferous fuels and crops based on Stockwell et al.[22, 23] and supplemented with GC×GC-TOFMS data from FLAME-IV.[24] The Stockwell et al.[22, 23] data are scaled to field MCE values; the GC×GC-TOFMS laboratory-based EFs were scaled relative to the Stockwell et al.[22, 23] methane emissions. Each of the individual compounds were then lumped into one of 34 MOZART-4[25] and one of 38 SAPRC-07[26] surrogate species based on the following: 1) estimated OH reactivity, and 2) oxidation product distribution ([27], IUPAC Atmospheric Chemical Kinetic Data Evaluation, http://iupac.pole-ether.fr/). This mapping to surrogates and the resulting speciation profile allow the explicit compounds identified during FLAME-IV to be modeled using simplified chemical mechanisms and lumped surrogate species within air quality modeling frameworks, including AIRPACT.

0-D Modeling

This section describes the 0-D modeling approaches, including development of mechanisms and parameterizations for SOA formation and processing. Monoterpenes and furan/furan derivatives were the two compound classes that were selected for the box modeling efforts. For the monoterpenes, though SOA formation has not been studied for a diverse number of specific compounds, enough information about their general reactivity exists such that they can be treated robustly in a semi-explicit model. We used the model, GECKO-A (Generator of Explicit Chemistry and Kinetics of Organics in the Atmosphere), to predict SOA formation from different monoterpenes. GECKO-A has two components: an explicit chemical mechanism generator and an SOA box model.[28] The mechanism generator generates semi-explicit gas-phase oxidation mechanisms for individual compounds under general atmospheric conditions, while the SOA box model simulates SOA formation from individual precursors based on their generated reaction schemes.[28-30] In the absence of experimental data, reaction rate constants and/or products are estimated based on structure/activity relationships (SARs).[29] Gas-particle partitioning of those products is calculated assuming thermodynamic equilibrium with activity coefficients = 1. The SOA box model does not include representation of heterogenous/aqueous reactions in its current form, nor non-equilibrium partitioning. The modeling simulation results were fit using the volatility basis set (VBS) framework,[31] similarly to how one would fit chamber data using the same approach, to generate SOA modeling parameters. We note that JFSP funding was used to send a graduate student to train directly with the developers of GECKO-A. Outside of the developers, we are the first group to run GECKO-A, and the first to apply it for analysis of SOA formation from BB-derived precursors.

The other class of prioritized compounds, furan/furan-derivatives, could not be robustly represented using GECKO-A due to the lack of existing data/reliable SARs for such compounds. Therefore, we leveraged this JFSP project to start another project to provide the fundamental information ultimately required to develop the detailed models from which parameterizations can be derived. With that funding, we developed a chemical mechanism for furan/methylfurans in SAPRC. This will be published soon and available for application in CMAQ and other models.

This project also sought to evaluate non-traditional mechanisms for SOA formation (e.g., heterogeneous reactions, including accretion, and oxidation of lower volatility precursors).

Consideration of the oxidation of lower volatility precursors was achieved by first identifying the relevant precursors, and then treating them in chemical mechanism models as described above. Heterogeneous reactions can be treated with varying levels of complexity. The latest CMAQ model (v.5.2) has a highly simplified mechanism built in that converts gaseous organic carbon to particulate organic carbon, which represents all such non-traditional mechanisms for SOA formation. For wildfires, this is only applied to evaporative emissions of primary OA.[32] Thus, a single volatility distribution for all combustion primary OA is assumed, and a fraction of the gaseous carbon (following dilution) is oxidized to form lower volatility compounds using a fixed rate constant. We developed a framework that also allows consideration of non-traditional mechanisms, which can work on individual compounds or lumped surrogates.[33] We presented a set of equations that can be used to describe the contribution of monomers vs. accretion products (dimers) to SOA formation. The formation of dimers serves to reduce the effective volatility of the monomer, thus promoting SOA formation. This method requires knowledge of or estimation of the extent of accretion product formation. It was determined that at this time, there are not sufficient data to constrain these complex representations. They can be used to assess sensitivity, but should not be thought of as predictive at this stage and thus will not be further discussed.

Air Quality Modeling

The section describes the approach for the air quality model sensitivity studies. We used Washing State University's 3-D regional air quality modeling system for the Pacific Northwest (PNW) called AIRPACT,[34, 35] run at 4×4-km resolution with 37 vertical layers. The modeling framework utilizes SMARTFire and BlueSky[36] for fire information and emissions, respectively; MEGAN[37] for biogenic emissions; SMOKE[38] for anthropogenic emissions processing; WRF[39] for meteorology; and CMAQ[40] for atmospheric chemistry and transport.

The first set of AIRPACT modeling simulations was conducted for the period of August 2015 with CMAQv5.0.2 (April 2014 release). The modeling simulations were then redesigned to use the latest version of CMAQv5.2 (June 2017 release), which has a significantly revised SOA formation module; and to better represent plume height and total organic carbon emissions (gaseous and particulate). In addition, the modeling simulations were conducted for the period of August 2013, in which there was a much more complete set of observational data with which to compare the model simulations. The revised modeling approach required resetting of emissions, meteorology inputs, and boundary chemical conditions. Predicted SOA, primary OA, and $PM_{2.5}$ levels were then compared with observations of total PM and total OA. Table 1 below lists the base and sensitivity simulations performed with CMAQv.5.2.

Table 1: Description of AIRPACT w/CMAQv. 5.2 Sensitivity Simulations

	Gaseous NMOCs		**$PM_{2.5}$**	
Fire Emissions Scenarios	**Emission Factor**	**Speciation Profile**	**Emission Factor**	**Speciation Profile**
BASE	Default (32.4 g/kg)	Default	Default (12 g/kg)	Default
SENS1	× 1.54	Updated	Default	Default
SENS2	× 1.54	Updated	× 2.23	Default
SENS3	× 1.54	Updated	× 2.23	Updated

Results and Discussions

Emission Factor Data Compilation and Analysis

Relevant Objectives: 1, 2, 3

All of the individual compounds measured during FLAME-IV and included in the comprehensive gaseous NMOC EF database, developed in this project, were binned by estimated saturation vapor concentration (C^*); an example of the resulting EF volatility distribution is shown in Fig. 1 for ponderosa pine smoke (for other fuels see Hatch et al. [1]). The volatility of compounds spans 9 orders of magnitude; 7 of which contain significant mass. Relative to the other fuels, the pine smoke sample had the largest fraction of IVOCs, ~11% of the total gaseous NMOC EF (6-8% for the other fuels). For comparison, compounds typically measured in BB smoke (based on Table 1 in Akagi et al.[10]) and those included in the EPA SPECIATE emission inventory [41] are also included in Fig. 1. The volatility of the typically measured compounds and those in the SPECIATE emissions inventory span 8 orders of magnitude; however compounds in only 5 bins contribute significantly to the overall EF in both cases.

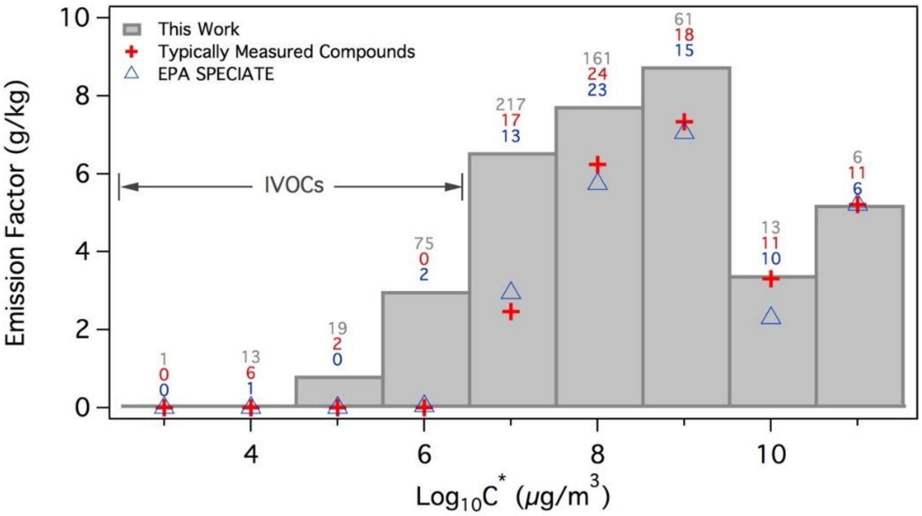

Figure 1: Emission factors of gaseous non-methane organic compounds determined in pine smoke, as a function of volatility. Red (+) and blue (Δ) markers indicate the contribution from typically measured compounds based on (Akagi et al., 2011 [8]) and the EPA SPECIATE emission inventory [39]; numbers indicate the number of compounds in each bin.

Emission inventories are used in air quality models to distribute the total gaseous NMOC among the suite of compounds included in the inventory; which are then mapped to lumped model species for treatment in gas-phase chemical mechanisms and SOA modules. Since the fraction of each bin accounted for by the SPECIATE inventory decreases with decreasing volatility (Fig. 1), application of the SPECIATE inventory would result in a group of model compounds with a significantly higher mean volatility than the application of our new inventory. In particular, IVOCs were almost entirely absent; less than ~1% of the IVOC EF we measured for pine smoke was accounted for by the compounds included in the Akagi et al. compilation (based primarily on field studies)[8] and the SPECIATE inventory.

We were able to identify and quantify a large fraction of the unspeciated mass highlighted by the Akagi et al.[10] compilation. For the top 100 compounds from each fuel, which account for ~90% of the total gaseous NMOC EF for each fuel (87-91%), the measured EF was scaled by the corresponding rate constant for reaction with OH to determine the most reactive compounds and by carbon number as a rough proxy for total potential SOA contribution. These scaled EFs were termed ‘reactive carbon’. Compounds were then sorted by the number of publications reporting an SOA yield via OH-radical oxidation (as of May 2016). Results are shown in the Figs. 2 and 3 for pine and black spruce smoke, respectively, illustrating that only 12-22% of the reactive carbon is associated with very well studied compounds (5+ publications). In contrast, between 55% and 77% of the reactive carbon was associated with compounds for which SOA yields are unknown or understudied (0-1 publications). Of the understudied compounds, those most likely to form SOA are outlined in gray in the pie charts of Figs. 2 and 3. Thus one important finding is that even with the improved speciation measurements and compilation of a comprehensive EF database, critical data for modeling BB SOA formation are missing for a significant fraction of the potentially reactive material.

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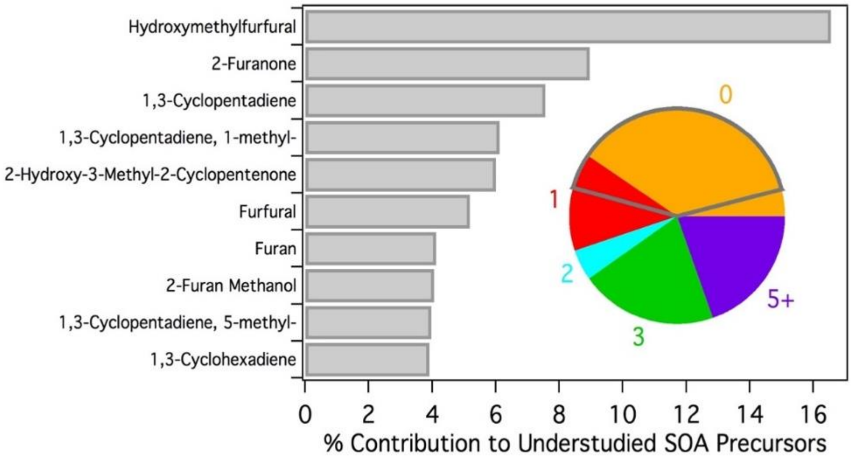
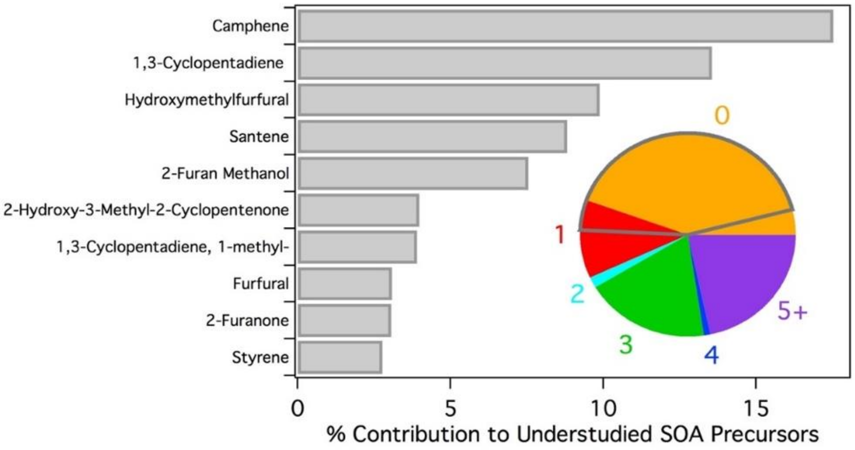


Figure 2: Assessment of SOA yields for compounds detected in the ponderosa pine fire. Pie chart: Classification of reactive carbon (see text) by the number of publications reporting an SOA yield following hydroxyl radical oxidation. The gray-outlined wedge represents the understudied compounds with the greatest potential to form SOA. Bar chart: Percent contribution of the top 10 compounds included in the gray wedge.

Figure 3**:** Same as above for black spruce.



Many of the understudied potential precursors are furan derivatives and polyunsaturated aliphatic hydrocarbons; only ~10% to 28% of the reactive carbon contributed by understudied precursors is attributed to aromatic compounds. Thus the largest gaps in known SOA yields relevant for BB are associated with non-aromatic compounds (furans notwithstanding). To better identify specific candidates for future smog chamber studies, the top 10 understudied potential precursors are shown in the corresponding bar charts as a percentage of the reactive carbon included in the gray-outlined wedge (Figs. 2 and 3 for pine and black spruce, respectively; see Hatch et al. [1] for other fuel types). Given the ubiquity and potential importance of these compounds, future smog chamber experiments with these species may significantly help to narrow knowledge gaps regarding SOA yields of organic compounds in BB emissions.

Relevant Deliverables

Deliverable 1: EFs for FLAME-IV fuels as a function of burn and fuel characteristics. The FLAME-IV EFs largely were evaluated as a function of fuel type. The advantages of combining data from a number of instruments outweighed evaluating fewer samples (limited by overlapping data). With such a limited number of samples, EFs could not be sufficiently evaluated as a function of MCE. However, Stockwell et al.[20,21] and others have shown robust relationships between MCE and EF for a number of gaseous NMOCs. In recent work (unpublished), we have found that the relationship between MCE and EF can be complicated by diversity in fuel characteristics (e.g., canopy vs. woody debris) and particle loading (i.e., gas-particle partitioning of I/SVOCs).

0-D Modeling

Relevant Objective: 3

SOA from ten monoterpene precursors, including camphene, was modeled using GECKO-A. These modeling studies represent the first studies of SOA formation from camphene, which was one of the dominant monoterpenes in black spruce emissions (and also significant in other coniferous fuels). Atmospheric variables and initial conditions were defined to represent a "typical" chamber study, since chamber studies are widely used to evaluate the potential for individual precursors to form SOA and to develop SOA model parameterizations. Atmospheric variables were set as follows: temperature = 298K; relative humidity = 5%; aerosol seed = 1 µg m^{-3}; and solar zenith angle (required to compute the photolysis frequencies) = 50^{o}. The initial concentrations of precursor and oxidants were as follows: monoterpene = 50 ppb, NO = 50 ppb, formaldehyde = 50 ppb, and ethane = 10 ppm. We note that formaldehyde and ethane are not typically added in chamber studies; however, they control the gas-phase reactivity of compounds (and as such, the simulations are more able to represent the atmospheric reactivity of emitted compounds, particularly those that are less reactive). The formaldehyde and ethane do not directly participate in SOA formation (with the exception of generating oxidants).

The left two panels in Fig. 4 illustrate predicted SOA formation for camphene (pink trace), α-pinene (green trace), and limonene (orange trace). The top left panel illustrates SOA mass as a function of time. Limonene is known to have one of the highest (if not the highest) SOA yields among studied monoterpenes. Camphene is predicted to form significant amounts of SOA in these controlled reactivity simulations. The bottom left panel illustrates SOA mass as a function of reacted precursor concentration. Such plots are useful for evaluating the relative volatility of the predicted products, as oxidation products with lower volatility will start to form SOA at lower reacted hydrocarbon levels. Interestingly, camphene is predicted to form the lowest volatility precursors.

SOA mass formation vs. reacted hydrocarbon concentration are needed to develop SOA parameterizations using the VBS approach. We ran another ten simulations for each monoterpene precursor over a range of initial precursor concentrations and used the maximum predicted SOA concentration at each reacted hydrocarbon concentration to optimize VBS parameters (a minimum of four simulations are needed for each parameterization). The volatility bins are constrained by the predicted SOA concentrations. We chose a 5 bin VBS representation (C^* = 0.01-100), but this choice is flexible and can be modified to best fit the chosen air quality model framework.

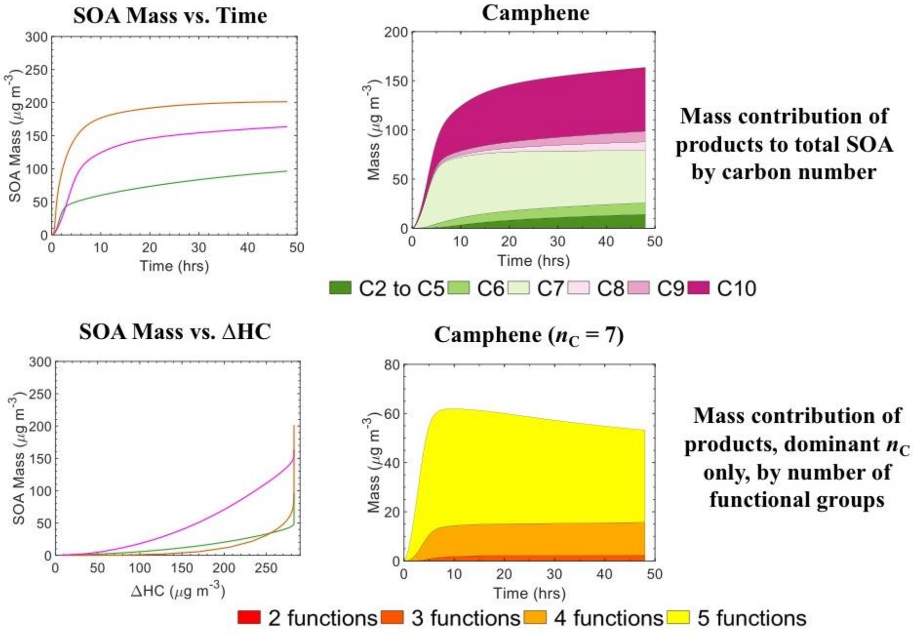


Figure 4: Predicted SOA formation for camphene (pink trace), α-pinene (green trace), and limonene (orange trace) using GECKO-A, as a function of time (top left) and reacted hydrocarbon (bottom left); particle phase composition of camphene SOA as a function of carbon number (top right) and number of functional groups (bottom right).

Since evaluation of SOA mass alone can be misleading from the perspective of model validation, we also examined the properties of the predicted particle-phase compounds, which can be compared with measurements as they become available. The top right panel in Fig. 4 illustrates the predicted mass contribution of products with 2 to 10 carbon atoms from camphene oxidation. Interestingly, the model predicts that compounds with 7 and 10 carbon atoms contribute the most to SOA. In the bottom right panel, the mass contribution of carbon number (n_C) = 7 compounds by the number of functional groups is shown for camphene. The model predicts a large number of compounds with 5 functional groups, which would have low volatility and thus support the observations from the lower left panel.

Relevant Deliverables

Deliverable 2: Evaluation of SOA formation from newly identified S/VOC precursors. The GECKO-A model is an excellent tool for evaluating SOA formation via oxidation from some of our newly identified precursors. Monoterpenes are particularly well represented in GECKO-A. Some of the other classes of compounds (e.g., furans) can not be well represented in GECKO-A at this time. We are evaluating approaches for also considering heterogeneous pathways for SOA formation using GECKO-A.

Deliverable 3: Parameterizations for SOA models. VBS parameterizations can be easily derived using an optimization algorithm from the GECKO-A model predictions. We have developed VBS parameters for ten monoterpenes, including camphene. The parameterizations are highly sensitive to initial conditions. We are now working to optimize our simulations to best represent ambient and fire conditions; from these simulations will we develop and publish our derived SOA parameters.

Air Quality Modeling

The inclusion of the newly identified and quantified NMOCs markedly changes the speciation profiles of the lumped model surrogates, as shown in Fig. 5. In panels a and b, each of the MOZART-4 surrogate species is represented by a colored wedge; only the top 5 (by mole fraction) are labeled. The offset wedges indicate a surrogate species with >3 carbon atoms (>C3 aldehydes, alkanes and alkenes; benzene; toluene; xylene; monoterpenes; isoprene; methyl ethyl ketone; methacrolein, phenol, xylol, and cresol). The updated profile (Fig. 4b) has a higher percentage of >C3 compounds, particularly >C3 alkenes (“BIGENE”) and lumped monoterpenes. It is expected that such changes in the NMOC distribution (as represented by the MOZART-4 surrogates), would result in changes in chemical production rates and concentrations of compounds of interest from

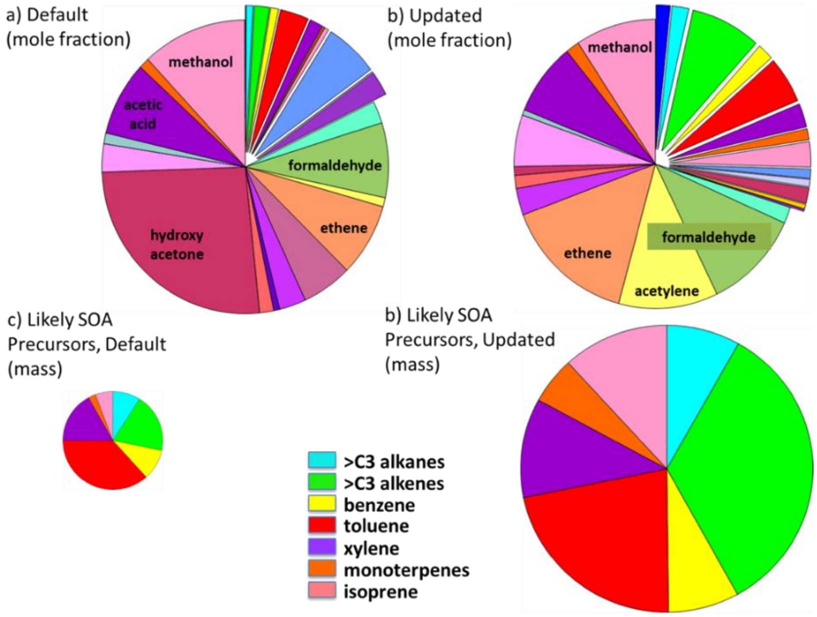


Figure 5: Speciation profile for coniferous fuels: a) default emissions inventory, b) updated emissions inventory, c) default-likely SOA precursors, and d) updated-likely SOA precursors. In panels a and b, surrogate compounds are represented as percentages of the total speciation profile; in panels c and d, surrogate compounds are represented as moles of species per area burned and pie charts are scaled to illustrate relative mass amounts.

an air quality and climate perspective. This may be better evidenced by the results in panels c and d. Panels c and d illustrate the relative mass fractions of those surrogates that are likely SOA precursors in the default (Fig. 4c) versus updated (Fig. 4d) profiles. In the MOZART-4 CTM benzene, toluene, xylene, monoterpenes, and isoprene serve as SOA precursors. While the >C3 alkanes and alkenes do not serve as SOA precursors in MOZART-4, 5% (by EF) of the >C3 alkane and 15% (by EF) of the >C3 alkene surrogates have carbon numbers > 10 and are thus likely to form SOA (e.g.,[18]). The updated profile has a factor of ~3 greater total mass allocated to likely SOA precursors. While the updated speciation profiles are shown for the MOZART-4 gas-phase chemical mechanism, the results look very similar for the SAPRC gas-phase chemical mechanism, which was used in the AIRPACT model simulations. Speciation profiles are available for MOZART-4 and SAPRC, based on our compiled EF database for coniferous fuels and crops.

SOA and $PM_{2.5}$ were predicted using the AIRPACT modeling framework with CMAQv.5.0.2 and CMAQ v.5.2. Fig. 6 illustrates predicted SOA (left panels) and PM2.5 (right panels) using the default SPECIATE emissions inventory (top panels) and our updated emissions inventory (bottom panels) with CMAQ v.5.0.2. The simulation period covers August 2015; active fires are shown as red spots in the middle figure. As can be seen in the left panels, the predicted SOA concentrations increase with the updated emissions; the maximum SOA increases by a factor of 2. However, as can be seen in the right panels, the predicted $PM_{2.5}$ is statistically similar and the negative bias in the model predictions is not mitigated. Further investigation and comparison with model results demonstrated that CMAQv.5.0.2 was significantly underestimating the contribution of SOA to $PM_{2.5}$, and thus the relative insensitivity to changes in predicted SOA concentrations.

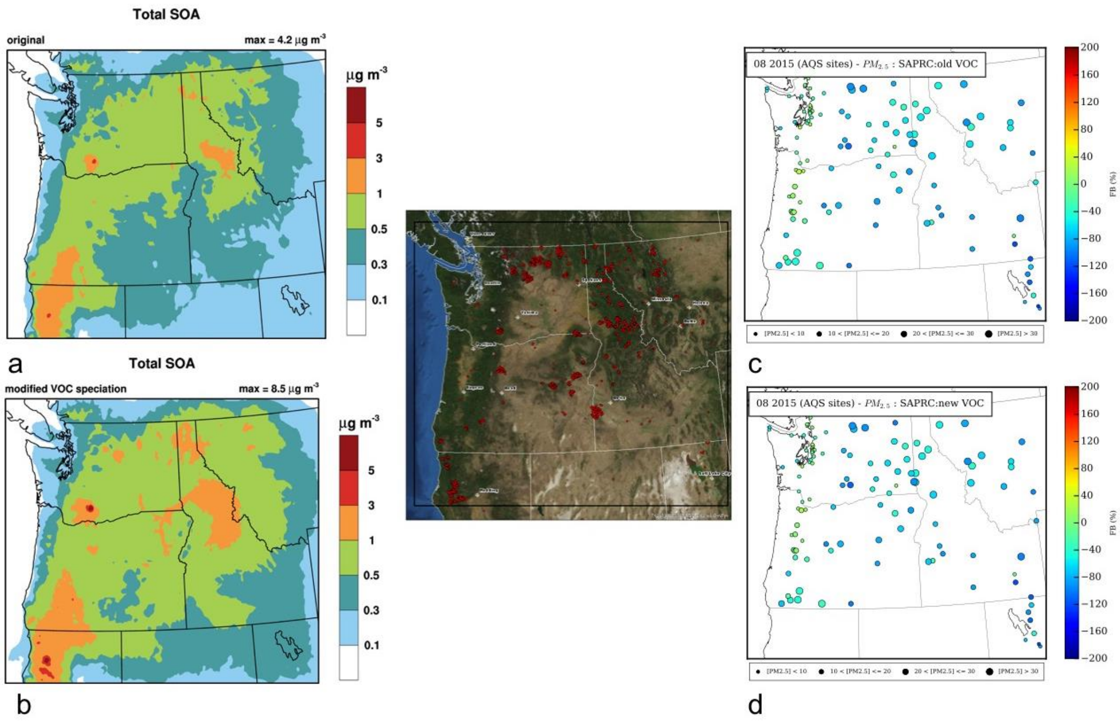


Figure 6: Predicted SOA and $PM_{2.5}$ using CMAQv.5.0.2 in AIRPACT.

Fig. 7 illustrates predicted $PM_{2.5}$ concentrations (circle size) and model bias (color scale) using the default SPECIATE emissions inventory (left panel) and our updated emissions inventory (right panel) with CMAQv.5.2. The sensitivity case also includes an increase in total NMOC emissions and fractional contribution of organic carbon to $PM_{2.5}$ (see Table 1) based on Liu et al.[2] The simulation period covers August 2013, in which observations from the BBOP field campaign were available. With the model updates in CMAQv.5.2, the overall negative bias is reduced, and at many sites there is an overprediction of $PM_{2.5}$. However, CMAQv.5.2 better represents the contribution of BB-derived SOA to total $PM_{2.5}$.

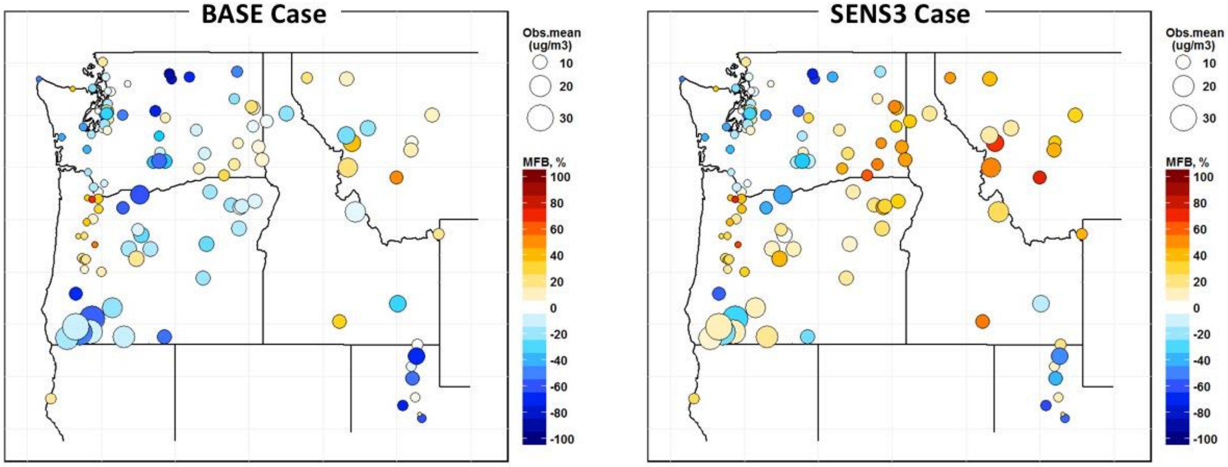


Figure 7: Predicted SOA and $PM_{2.5}$ using CMAQv.5.0.2 in AIRPACT.

Relevant Deliverables

Deliverable 4: Modifications and/or additions needed in emissions inventories and SOA models to better represent SOA from wildland fires. The updated EFs and associated speciation profiles significantly increased predicted SOA, and in CMAQv.5.2, also $PM_{2.5}$. Further measurements and model development are needed to refine parameterizations and minimize model bias.

Scientific Delivery

This final project report represents the efforts of all three principal investigators (Barsanti, Lamb, and Yokelson), as well as two graduate students, two postdocs, and two faculty (Chung, Lee) that were involved over the course of the project. We published a total of two core manuscripts (with one additional manuscript under review), and one with JFSP collaborators. Two additional manuscripts are in preparation. We gave 10 presentations at scientific conferences (8 talks + 2 posters), and collaborators gave another 5 presentations. We held two in-person workshops. Finally, PI Barsanti gave 5 additional presentations. One of these presentations kicked-off a Forest & Fire Learning series, hosted by the Mountain Studies Institute in Durango, CO; the other was followed by a panel discussion, which included wildland firefighters and land managers, hosted by the San Juan Headwaters Forest Health Partnership in Pagosa Springs, CO.

Key Findings and Implications for Management/Policy and Future Research

Field measurements (e.g., BBOP, Zhou et al.[3], Liu et al.[2]) and comparison of these observations with regional air quality models clearly demonstrate that a large fraction of primary $PM_{2.5}$ emitted from fires is organic and that a large fraction of $PM_{2.5}$ in fire-impacted regions contains a significant fraction of secondary organic aerosol (SOA). For this project we assembled a multidisciplinary team to perform an integrated analysis specifically of the importance of missing SOA precursors and processes on model-predicted $PM_{2.5}$ from wildland fire emissions. As the name suggests, SOA is a secondary pollutant formed through oxidation of gaseous organic precursors and multiphase reactions of the oxidation products. The relative contribution of SOA to $PM_{2.5}$ can influence the spatial and temporal distribution of $PM_{2.5}$ as well as the air quality and climate impacts. Thus, accurate representation of SOA formation from wildland fires is important to both fire and air quality management communities.

As step one, we performed/compiled the most extensive and detailed speciated measurements of gas-phase emissions of organic gases emitted by fires to date. This confirmed that a large number of important SOA precursors are not being represented in current air quality models, including AIRPACT (Obj. 1 and 2). We found that the quantities of gas-phase organic compounds, especially those that are of lower volatility and important SOA precursors, may be significantly underestimated in models by using EFs that are not scaled based on the gas-particle phase distribution (Obj. 1 and 3). We used a comprehensive screening procedure to show which of the newly identified compounds were likely to form significant SOA (Obj. 2). For several of these key precursors we used advanced box model simulations to explore their SOA yield and the associated chemical mechanisms. However, for most of the newly identified compounds, the lack of a known reaction mechanisms and SOA formation yields precluded completely explicit representation and development of parameterizations for AIPACT.

Development and validation of model parameterizations, including those used to represent the formation of SOA in air quality models, requires a significant investment of resources. Therefore it was important for us to evaluate the sensitivity of predicted $PM_{2.5}$ to changes in predicted SOA, and the extent to which improvements in the model representation of SOA precursors and processes improved predictions of $PM_{2.5}$ (Obj. 4-6). We found that model predictions of SOA formation were highly responsive to our upgraded fire emissions, but the $PM_{2.5}$ response depended strongly on the details of the SOA modules (i.e., the version of CMAQ used, 5.0.2 vs. 5.2). When coupled with our updates to wildland fire emissions, AIRPACT with CMAQv5.2 better reproduced the field-measured contribution of SOA to $PM_{2.5}$. The number of sites with negative biases in $PM_{2.5}$ was decreased; while the number of sites with positive biases increased. Thus, including the new precursors and processes improved SOA and $PM_{2.5}$ predictions, but further refinements and constraints are needed.

In summary, given the contribution of fire-derived SOA to $PM_{2.5}$ and model sensitivity of $PM_{2.5}$ predictions to both SOA precursors and parameterizations; further mechanistic data, field validation, and parameterizations are still needed for air quality models (Obj. 6). With these additional steps, more accurate representation of SOA formation from wildland fires can likely be achieved.

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Appendix B: List of Completed/Planned Scientific/Technical Publications/Science Delivery Products

Peer-Reviewed Journal Articles

Published

Barsanti, K., Kroll, J., Thornton, J. The formation of low-volatility organic compounds in the atmosphere: Recent advancements and insights. *Journal of Physical Chemistry Letters Perspective* (invited). 2017

Hatch, L.E., Yokelson, R. J., Stockwell, C.E., Veres, P. R., Simpson, I. J., Blake, D. R., Orlando, J. J., Barsanti, K. C. Multi-instrument comparison and compilation of non-methane organic gas emissions from biomass burning and implications for smoke-derived secondary organic aerosol precursors. *Atmospheric Chemistry & Physics*, 17: 1471, 1489. 2017

Bian, Q., Jathar, S. H., Kodros, J. K., Barsanti, K. C., Hatch, L. E., May, A. A., Kreidenweis, S. M., Pierce, J. R. Secondary organic aerosol formation in biomass-burning plumes: Theoretical analysis of lab studies and ambient plumes. *Atmospheric Chemistry & Physics* doi:10.5194/acp-2016-949

In Review

Ahern, A., Robinson, E., Tkacik, D., Saleh, R., Hatch, L., Barsanti, K. Stockwell, C., Yokelson, R., Presto, A., Robinson, A., Sullivan, R., Donahue, N. Production of secondary organic aerosol during aging of biomass-burning smoke from fresh fuels and its relationship to VOC precursors. *Journal of Geophysical Research-Atmospheres*, 2018JD029069

In Preparation

Afreh, I., Aumont, B., Camredon, M., Valorso, R., Barsanti, K. Predictions of SOA Formation and Composition from Camphene using GECKO-A.

Jiang, J., Carter, W.P., Cocker III, D.R., Hatch, L., Barsanti, K. Developing the SAPRC Gas-Phase Chemical Mechanism for Furan and Methylfurans.

Conference Proceedings

Barsanti, K., Hatch, L., Wiedinmyer, C., Orlando, J., Knote, C., Emmons, L., Stockwell, C., Yokelson, R., Veres, P. Evaluating Complexity in Fire Emissions Modeling: Is More Better? 21st Annual Emissions Inventory Conference, Sand Diego, CA. April 2015. Extended Abstract: https://www3.epa.gov/ttn/chief/conference/ei21/session10/barsanti.pdf

Conference Abstracts

Afreh, I., Aumont, B., Camredon, M., Valorso, R., Barsanti, K. *Developing Model Surrogates for Monoterpenes to Improve Predictions of Secondary Organic Aerosol*. 10th International Aerosol Conference, St. Louis, MO, September 2018. Abstracts: http://aaarabstracts.com/2018IAC/AbstractBook.pdf

Hatch, L., Liu, Y., Rivas Ubach, A., Shaw, J., Lipton, M., Barsanti, K. *Advanced Characterization of Semi-Volatile Compounds Emitted from Biomass Burning.* American

Geophysical Union Fall Meeting, New Orleans, LA, December 2017. Abstracts: https://agu.confex.com/agu/fm17/meetingapp.cgi/Person/51266

Nergui, T., Lee, Y., Chung, S. H., Lamb, B. K., Yokelson, R. J., and Barsanti K.: Integrating measurement based new knowledge on wildland fire emissions and chemistry into the AIRPACT air quality forecasting for the Pacific Northwest, AGU Fall Meeting Abstracts, December 2017. Abstracts: https://agu.confex.com/agu/fm17/meetingapp.cgi/Paper/224705

Barsanti, K., Hatch, L., Afreh, I., Aumont, B., Camredon, M., Orlando, J., Wiedinmyer, C. *Integrating Biomass Burning Emissions Measurements and Predictive Models of Secondary Organic Aerosol Formation*. International Aerosol Modeling Algorithms Conference. Davis, CA, December 2017.

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Led by Collaborators

Pierce, J. R., Bian, Q.-J., Kreidenweis, S. M., Kodros, J. K., Jathar, S., May, A., Hatch, L., Barsanti, K. *Investigation of particle and vapor wall-loss effects on controlled wood-smoke smog-chamber experiments*. 5th International Fire Behavior and Fuels Conference, Portland, OR, April, 2016

Bian, Q., Jathar, S., Kodros, J., Barsanti, K., Hatch, L., May, A., Kreidenweis, S., Pierce, J. *Secondary organic aerosol formation in biomass-burning plumes: Theoretical analysis of lab studies*. American Association of Aerosol Research Annual Conference, Portland, OR, October, 2016

Bian, Q., Pierce, J. R., Kodros, J. K., Kreidenweis, S. M., Jathar, S., May, A., Barsanti, K., Hatch, L., International Smoke Symposium, *Secondary organic aerosol formation in biomass-burning plumes: Theoretical analysis of lab studies*. Long Beach, CA, November, 2016

Pierce, J. R., Bian, Q.-j., May, A., Jathar, S., Kodros, J. K., Barsanti, K., Hatch, L., Kreidenweis S. M., "Exploring the evolution of biomass-burning aerosol in chambers and the atmosphere", University of Colorado (Invited Seminar), Chemistry, October 2016.

Kreidenweis, S. M., Pierce, J. R., Bian, Q.-j., May, A., Jathar, S., Kodros, J. K., Barsanti, K., Hatch, L., "Biomass burning aerosol: Emissions, evolution, and atmospheric impacts," seminar to be presented in the William G. Lowrie Department of Chemical and Biomolecular Engineering, The Ohio State University, September 7, 2017

Posters

Jiang, J., Carter, W.P., Cocker III, D.R., Hatch, L., Barsanti, K. *Developing the SAPRC Gas-Phase Chemical Mechanism and Chamber-Based SOA Parameterizations for Evaluating Biomass-Burning Derived SOA from Furan and Furan Derivatives*. 10th International Aerosol Conference, St. Louis, MO, September, 2018

Afreh, I., Aumont, B., Camredon, M., Valorso, R., Barsanti, K. *Development of Model Surrogates for Monoterpenes to Improve Predictions of Secondary Organic Aerosol.* Gordon Research Conference (GRC), Les Diablerets, Switzerland, June 2018

Presentations/Webinars/Other Outreach

Afreh, I., Aumont, B., Camredon, M., Valorso, R., Barsanti, K. *Development of Model Surrogates for Monoterpenes to Improve Predictions of Secondary Organic Aerosol.* Gordon Research Seminar (GRS), Les Diablerets, Switzerland, June 2018

Barsanti, K. *Managing Chemical Complexity in Predictive Models of Secondary Organic Aerosol*. Informal Symposium on Kinetics and Photochemical Processes in the Atmosphere. Pasadena, CA, March 2018 (invited speaker)

Barsanti, K. *Smoky Air: Should We Care?* Two keynote presentations: 1.. San Juan Headwaters Forest Health Partnership, Pagosa Springs, CO, March 2018 (presentation and panel discussion); 2. Mountain Studies Institute Durango, CO, March 2018 (presentation)

Barsanti, K. *Understanding Impacts of Wildfires and Vehicles to our Environment and Health.* UCR Board of Trustees. Riverside, CA, February 2018

Barsanti, K. Berkeley Atmospheric Science Center Seminar. *Embracing Chemical Complexity in Biomass Burning Emissions and Mechanistic Models*. Berkeley, CA, February 2017

Barsanti, K. Department of Atmospheric Sciences Seminar, Colorado State University. *Exploring Chemical Complexity in Biomass Burning Emissions and Air Quality Models*. Fort Collins, CO, March 2016