We thank the reviewer for his/her comments on our paper. To guide the review process we have copied the reviewer comments *in black italics*. Our responses are in regular blue font. We have responded to all the referee comments and made alterations to our paper (existing manuscript text **in bold text,** new/altered parts additionally **highlighted in yellow**).

Reviewer #1

Knote et al perform a sensitivity analysis to evaluate the impact of uncertainties in dry and wet deposition of SVOCs on SOA model predictions. They use the WRF-Chem model implemented with the VBS SOA formation scheme for this analysis. Recent work has suggested that Henry's law constants for SVOC species may be substantially larger than what is typically used in models meaning that deposition would be enhanced. Knote et al, implement these new higher Henry's law constants and evaluate their impact on wet and dry deposition separately and together. Due to the large uncertainty in this parameter they also conduct a series of sensitivity analyses using different Henry's law constants, different SOA aging rates, and different reactivity factors. They find that the use of the higher Henry's law constant can reduce SOA concentrations by 50% compared to no deposition of SVOCs, mostly due to enhanced dry deposition. This study addresses an important uncertainty in modeling SOA concentrations that has not previously received a great deal of attention. I have some suggestions for improvements, but recommend publication after revisions.

General comments:
Discussion of emissions on page 13736 and 13738: Emissions inputs have a large impact on any VBS results so it is essential to have a full description of what emissions were used in order for the reader to properly understand the results. The authors should add details on the emissions used including:

R1.1 On page 13736, line 1, the authors mention mapping of SAPRC99 species to MOZART species but do not mention that the AQMEII emissions were originally available as CB05. A similar table in the supplement should show how the CB05 species were first mapped to SAPRC99 species before the second mapping to MOZART species could take place.

The mapping from SAPRC to MOZART mentioned in the text refers to SOA yields as provided in Lane et al. (2008). These are not emissions, but rather reflect the amount of SOA formed per oxidation reaction of a certain precursor.

We agree with the reviewer that conversion tables for emission species are helpful to other modellers. We have added two tables to the supplement that detail the conversion of gaseous and particulate emissions from CB05 / AER06 to MOZART / MOSAIC respectively. These are now referenced in the text as:

Emission conversion tables for the MOZART/MOSAIC setup used in this work are given in Tables S1 / S2 in the supplement. The simulations are split into 48 h long chunks of free running meteorology [...]

The tables are also reproduced at the end of this document.

R1.2 Please specify whether the 2010 AQMEII emissions are based on the 2005 or 2008 NEI. Substantial changes to methods (including switch of mobile emissions model from MOBILE6 to MOVES) occurred between these two inventories so it is important to state what base-year NEI was used to derive the AQMEII emissions.

The section has been updated to include more information about emissions preprocessing. A separate publication detailing the preparation process (Pouliot et al., 2014, currently under review) has been referenced as well. The updated paragraph reads

[...] conducted within the MACC project. Emissions of trace gases and aerosols are those provided in phase 2 of the Air Quality Model Evaluation International Initiative model intercomparison (AQMEII, Alapaty et al., 2012). For the United States, the 2008 National Emission Inventory (NEI) (version 2, released April 10, 2012) was used (http://www.epa.gov/ttn/chief/net/2008inventory.html). Updates for the following activity sectors were applied to reflect changes in emissions between 2008 and 2010: on-/off-road transport, wildfires and prescribed fires, and continuous emission monitoring equipped point sources. Preparation of the emission data is described in detail in Pouliot et al. (2014). Emission conversion tables [...]

R1.3 Please describe how the organic emissions were apportioned to volatility bins. Were emissions of IVOCs and SVOCs included in these emissions? If so, what assumptions were used to derive these emissions since they were not part of the AQMEII emissions inputs? Many past VBS studies have apportioned POA emissions into different volatility bins and have assumed some additional IVOC/SVOC mass determined by applying a factor to the POA emissions (sometimes increasing POA emissions by up to a factor of 7.5 to account for “unmeasured” IVOC mass in the inventory). Were any such assumptions made here? The authors state that POA was *treated as non-volatile. If this is the case, then previously developed factors for increasing organic mass before distributing POA into volatility bins may not be appropriate here. If no IVOCs or SVOCs were emitted, then state this explicitly. If emissions for these species were derived, please describe and justify the methods used.*

We consider POA as a non-volatile species, and therefore POA is emitted into the particle-phase and does not partition between gas- and particle-phase. We did not emit any additional S/IVOC gases in our runs, as we assumed that they are already partially included in our inert POA. POA is however considered as additional particle-phase organic material in the pseudo-equilibrium calculations.

All SOA mass is formed through the oxidation of gaseous precursors such as isoprene, monoterpenes, benzene, toluene, and so forth. Oxidation products (by OH and O3) of these precursors are distributed according to their volatility into the VBS bins.

We already stated in the manuscript that POA is inert (p 13736, l 23-25). To emphasize that we don't include SVOC/IVOC emissions we extended this sentence, which now reads

Direct emissions of organic particulates (primary organic aerosols, POA) are included as inert contribution to aerosol mass without consideration of evaporation and re-condensation. Direct emissions of semi / intermediate volatility organic compounds (SVOC/IVOC) are not considered in this study.

R1.4 Please provide more description of the Hodzic et al results used to determine H. Since the new Hodzic et al. H* values are the basis for this work, more details are warranted. What specific compounds are used to create the weighted H* values for each volatility bin? Are these compounds primary VOC oxidation products or are they the result of multiple oxidation steps? Is it reasonable to believe that such highly soluble compounds would be found universally in all ambient aerosol across the United States or might their prevalence vary based on spatially varying meteorology (humidity, insolation rates etc) and emissions sources?*

As suggested by the reviewer we have provided a more detailed description of the solubility parameterization. H* values applied in this study were calculated by Hodzic et al. using the explicit chemical mechanism GECKO-A (Aumont et al., 2005) for the multi-generational oxidation products of individual SOA precursors. Values of H* were taken at the maximum of the SOA formation from each individual precursor, which is typically after 1-3 days of chemical processing (several steps of oxidation) depending on the precursor, and provided as a function of the volatility (VBS bins). In each volatility bin, a mass-weighted H* was calculated (see Table 1 in Hodzic et al. 2014). Using those values, we calculated in this study an averaged H* for both biogenic and anthropogenic precursor species. I.e. for biogenic species H* was averaged for isoprene and terpenes, whereas for anthropogenic species H* was averaged for short-chain alkanes and alkenes, and aromatics.

It is reasonable to consider that highly processed and oxygenated species (with 3-4 functional groups) will be highly soluble (Hodzic et al., 2013). The degree of chemical ageing/processing will of course depend on OH levels, as well as the type of precursors. As suggested by Hodzic et al., 2014, products of isoprene are typically more soluble than products of n-alkanes. The ageing that is considered in the VBS parameterization allows taking into account the amount of solar radiation through OH oxidation, and shifting the mass from volatile and less soluble VBS bins, into less volatile and more soluble ones. We acknowledge that large uncertainties still exist in the formation mechanisms of SOA (e.g. missing aqueous and in-particle phase reactions) that could impact the volatility of the oxidation products and our results, and we have tested the robustness of our results to changes in the volatility distribution.

This is now better explained on the manuscript:

Henry's law constants (H*, M atm^{-1}) used in this study for semi-volatile organic compounds were provided as a function of volatility by Hodzic et al. (2014a). They applied an explicit chemical mechanism (GECKO-A, Aumont et al., 2005) to generate the multi-generational oxidation products of individual SOA precursors and calculate the associated H* values using structure activity relationships (Raventos-Duran et al. 2010). Values of H* were taken at the maximum of the SOA formation from each individual precursor, which is typically after 1-3 days of chemical processing depending on the precursor, and provided as a function of the volatility (VBS bins). In each volatility bin, a mass-weighted H* was calculated (see Table 1 in Hodzic et al. 2014). Using those values, we calculated in this study an averaged H* for both biogenic and anthropogenic precursor species (Table 2). Dry and/or wet deposition of these volatile compounds is then considered by adding these species to the respective modules in WRF-Chem described above.

R1.5 The authors conduct simulations using the higher H values from Hodzic et al and compare those against simulations with no deposition. However, perhaps a fairer comparison would be the Hodzic H* values compared to more typical assumptions of H* in the photochemical models. I'd suggest that the authors conduct another sensitivity simulation using "traditional" H* assumption. For instance, acetic acid is used as a* *surrogate for dry deposition of SVOC vapors in the CMAQ model (H* = 4.1x10ˆ3) and adipic acid is used as a surrogate for wet deposition of SVOC vapors (see Carleton et al., 2010). Or, the authors could use the Ahmadov suggestion (0.25-0.5 times the HNO3 rate) for their "traditional" H* sensitivity. Comparing against "no dep" baseline is a bit of a strawman.*

The reviewer may have missed that simulations considering lower (but non-zero) Henry's law constants (H* = 1e5, H* = H*(HNO_3)) were already included and discussed in the manuscript (see the abstract, section 5.2, the conclusions, Figure 7, and Table 3). We showed that using H* = 1e5 leads to 25% and H* = H*(HNO_3) to 10 % overestimation of SOA concentrations vs. using the H* values derived in Hodzic et al., 2014. We agree with the reviewer that the simulation with no deposition is unrealistic, however it is a useful sensitivity case in that it provides an upper limit for quantifying the impact of this processus.

Given that the values for H* suggested by the reviewer are in between 0 and 1e5, the resulting overestimations will be between 50 and 25%. To estimate that value more precisely we conducted an additional simulation with H* = H* (CH_3COOH) (4.1e3, -dlnH/dlnT 6300, Johnson et al., 1996). This is now mentioned in the abstract

Assumptions about the water solubility of SVOCs made in some current modeling systems (H* = H*(CH_3COOH); H* = 10^5 M atm^{-1}; H* = H*(HNO_3)) still lead to an overestimation of 35% / 25% / 10% compared to our best estimate.

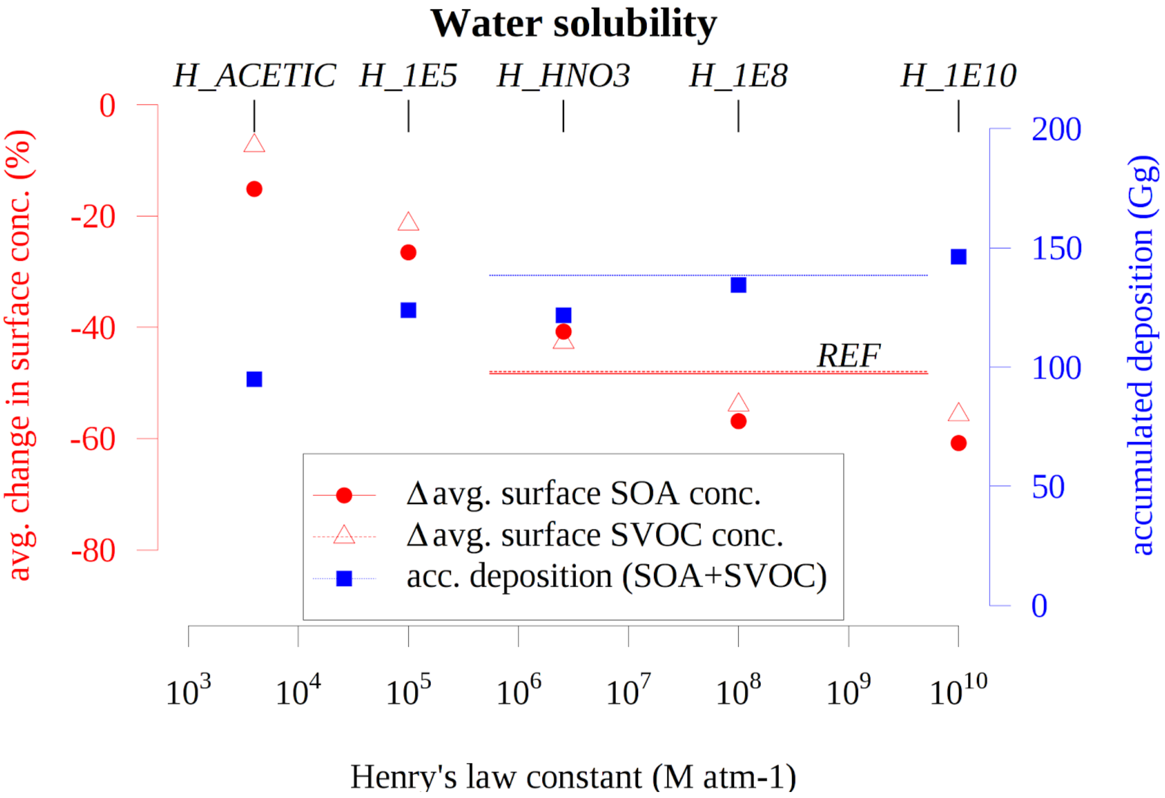
and in section 2.3

[...] but which are assumed to be very soluble. The fifth simulation (H_ACETIC) employs the Henry's law constant of acetic acid (CH_3COOH), as this is very similar to the values currently used in the Community Multi-Scale Air Quality Model (CMAQ, https://www.cmascenter.org/cmaq/, accessed July 18 2014). In the final two simulations [...]

and in section 5.2

[...] In these simulations we ignore the temperature dependence of the Henry's law constants. Additionally we included two simulations using Henry's law values derived for CH_3COOH (H* = 4.1 × 10^3 M atm^{-1} , d(ln H*)/d(1/T) = 6300) and HNO_3 (H* = 2.6×10^6 Matm−1, d(lnH*)/d(1/T) = 8700), commonly used in models as reference for very soluble compounds for which exact H∗ values are unknown. [...]

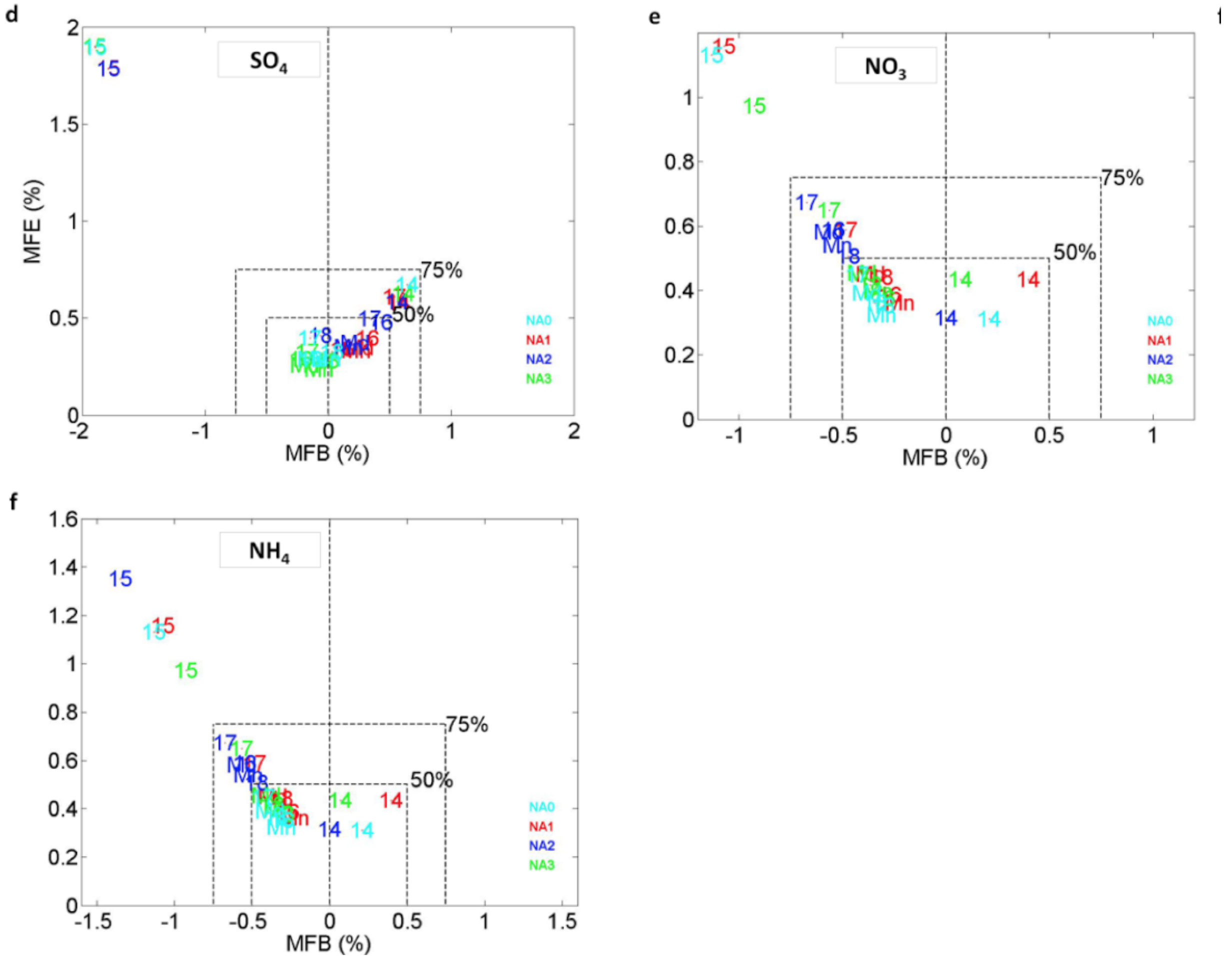
Figure 7 was updated accordingly:



The article would benefit from some more in depth model evaluation:
R1.6 Why is model performance for NH4 wet dep worse than either NO3 or SO4 wet dep? It seems like these should be related. Some exploration of this question is warranted. Wet deposition is an important endpoint, but looking at ambient concentrations may be more informative in terms of model performance. Consider adding analysis of IMPROVE ambient nitrate and sulfate concentrations (IMPROVE measurements of ammonium are only available at a limited number of sites for limited time periods). The CSN network measures all three compounds, but may be less appropriate here since that is an urban-focused network and the grid resolution (36 km) may be too coarse to capture urban gradients. The last sentence on lines 18-20 of page 13740 may be a bit of an overstatement: "The model results . . . shows that the underlying processes are accurately modeled . . ." Compensating errors cannot be ruled out without a more thorough model evaluation.

For a more general model evaluation and intercomparison would like to refer the reviewer to the upcoming results of the AQMEII phase 2 model intercomparison, in which the model system used in our work was employed in a very similar configuration (same parameterizations, grid and input data, only differing in the way SOA is formed and removed). Two manuscripts describe the model evaluation of O_3 and particulate matter (Im et al., 2014a, 2014b).

The following Figure (adapted from Figure 12 in Im et al., 2014b) is a “soccer plot” (Appel et al., 2011) showing the performance of different setups of WRF-Chem (NCAR, North Carolina State University, University of Murcia / Spain), WRF-CMAQ (U.S. EPA), and GEM-MACH (Env. Canada) when compared against a combination of CASTnet, IMPROVE and the US E.P.A. AQS data (http://www.epa.gov/ttn/airs/airsaqs/detaildata/downloadaqsdata.htm) (SO_4 at 250, NO_3 at 148, and NH_4 at 149 stations). Our model simulations are marked by the number 17. The results are further broken down into subregions (Im et al., 2014b) NA1 (southwest), NA2 (southeast), and NA3 (northeast). NA0 are statistics over all stations.



These results in particular and the overall results of AQMEII phase 2 show that our model performance is on par with the suite of state-of-the-art modeling systems participating in AQMEII phase 2. We agree with the reviewer that there might be compensating errors that we could not identify with the limited evaluation done in this work.

We note that NH_3 (and subsequently NH_4^+) modeling has been notoriously difficult for current modeling systems as there is evidence that a more sophisticated parameterization of the bidirectional surface <-> atmosphere flux than simple emission fluxes is needed (e.g. Nemitz et al., 2001; Bash et al., 2013).

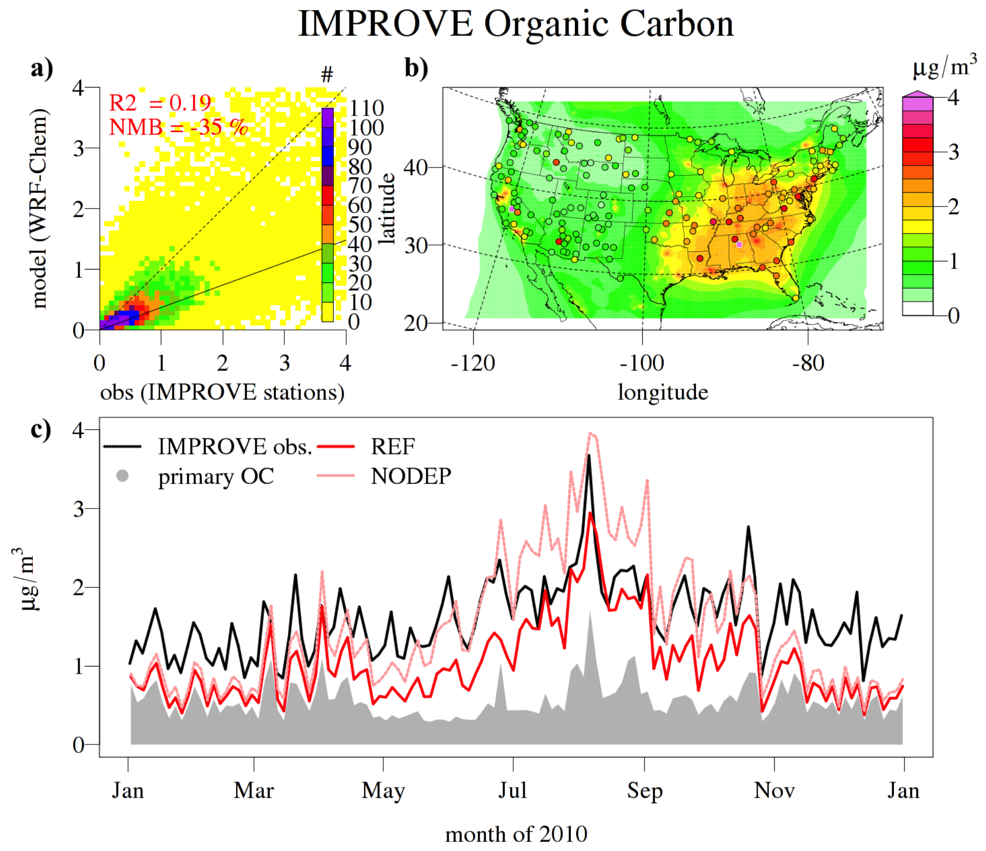
This discussion has been reflected in the text which now reads:

[...] wet deposition of ammonium is underestimated but still has a good correlation with measurements (R^2 = 0.69, NMB = −38). This deficiency could be related to the lack of a bi-directional exchange model in WRF-Chem to describe the flux of NH_3 at the surface (Nemitz et al., 2001; Bash et al., 2013). Measurements of water-soluble organics are not available so we could not directly evaluate the performance of WRF-Chem. The model results of wet deposition of inorganic ions however shows that the underlying processes are reasonably modeled, lending credibility to the accuracy of the wet deposition of organic substances.

R1.7 The spatial and temporal averaging used in evaluation of OC concentrations may mask model performance issues. Wintertime OC concentrations are likely dominated by POA while summertime OC concentrations are largely due to SOA. Consequently looking only at annual average values may make interpretation of results difficult. In figure 5 (top left), I suggest that rather than looking at the annual average at each monitor location, you include daily (24-hr avg) data in the scatterplot. If data are too dense to be distinguished on the scatter plot a density scatter plot could be used. The R2 and NMB metrics should definitely be calculated using daily data in addition to (or in place of) annual average data. The map might be more informative if it was created by season since the physical and chemical processes governing OC fate and transport are different in summer and winter. Perhaps include a map of summertime average in the main paper and maps of other seasons in the supplemental information.

We agree with the reviewer. We have accordingly modified Figure 5 (and added a new Figure 6, see R1.8). We now show a density scatterplot based on daily values. A scatterplot and map using only summer values has been added to the Supplementary Material, and is referenced in the revised text.

We identified an error in the plotting routine which erroneously showed SOA concentrations instead of POA concentrations as grey area in the time series, which is now corrected. This now even more clearly shows that wintertime is considerably more influenced by POA in the model as the reviewer already pointed out (see also our reply R1.18).



The revised figure caption now reads:

Evaluation of ground level total organic carbon (OC) concentrations against IMPROVE measurements. a) density scatterplot of daily average concentrations at each IMPROVE station against modeled concentrations (R^2 and NMB as defined in Fig. 3, again using the REF simulation). b) annual average OC surface level concentrations (REF simulation). Filled circles represent measured concentrations. c) time evolution of OC concentrations as average over all IMPROVE stations. Black solid line is measurement average. Grey area represents the POC contribution to total OC (from REF simulation). Light red and red lines are NODEP and REF simulation averages of total OC respectively.

R1.8 Spatial averaging used to create time series plots for figure 5 may also obscure spatially varying patterns. Consider grouping monitors into regions based on similar OC sources/concentrations (i.e. the OC in the Southeastern US is formed from different sources than the OC in the Northeast corridor or near Los Angeles). Consider creating time serious plots for each region to see if different patterns emerge in different areas. Since these results are the meat of the paper, it is worth exploring them in a little more depth.

We have created an additional Figure 6 in which we show the performance when compared in the 3 subregions of most interest: the West coast, the Northeast, and the Southeast (see below). This plot is now referenced in the text:

In the REF simulation with removals, the overall concentrations of OC are underestimated compared to measurements, but the month-to-month evolution is considerably more similar to the observed evolution. We further disaggregated the analysis spatially and looked at the performance at stations at the west coast, the Northeast and the Southeast (Fig. 6). Our findings show that on the west coast, modeled OC is underestimated in all simulations, while in the Eastern US, both REF and LOWVOL results track observed OC concentrations well during July and August, but underestimate them in June.

We further [...]

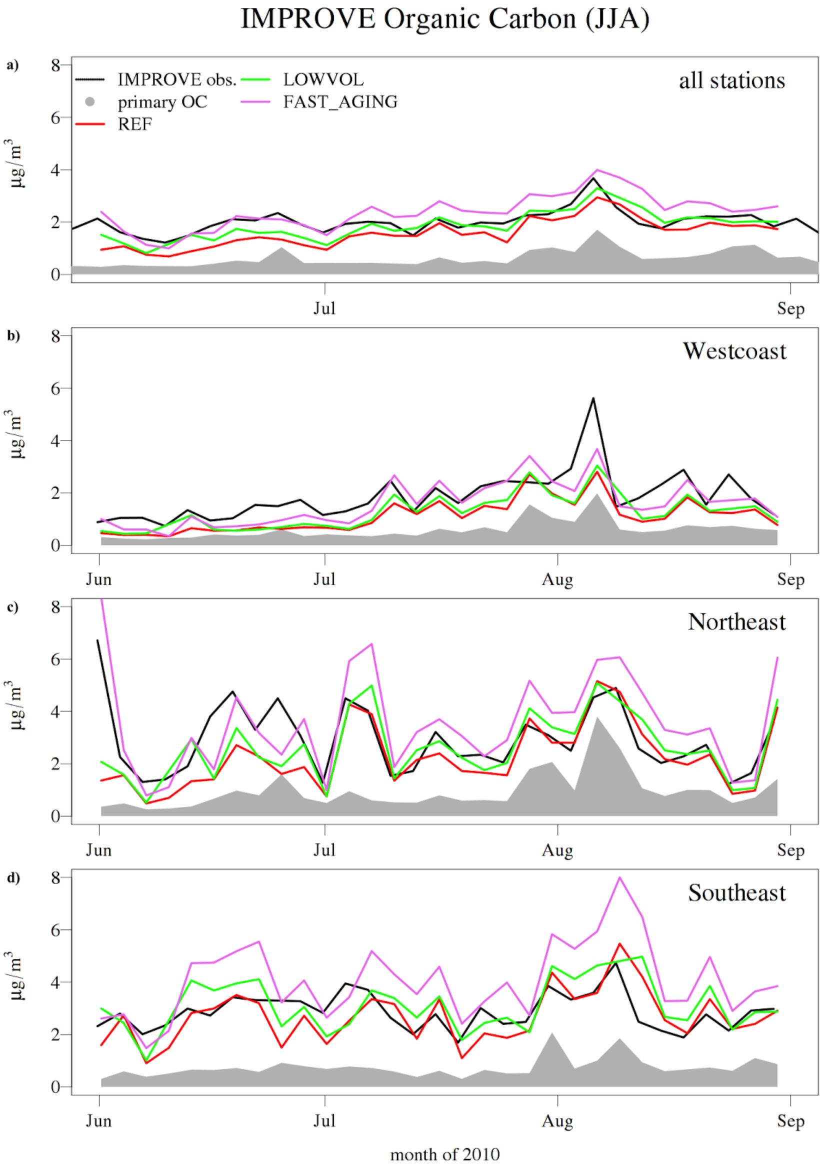


Fig. 6. Time lines of ground level total organic carbon (OC) concentrations against IMPROVE measurements like in Figure 5, but only for the summer period (June, July, August). Green and pink lines are for LOWVOL and FAST AGING sensitivity studies, respectively. a) all stations. b) west coast: California, Oregon, Washington. c) Northeast: Connecticut, Maine, Massachusetts, New Hampshire, Vermont, New Jersey, New York, Pennsylvania, Maryland, District of Columbia, Illinois, Indiana, Michigan, Ohio. d) Southeast: Alabama, Florida, Kentucky, Georgia, North Carolina, South Carolina, Tennessee, West Virginia, Virginia.

R1.9 It might also be interesting to look at the diurnal cycle of OC and how that is impacted by the deposition scheme. This may give some insight into whether the volatility of OC is being properly captured in the modeling. I believe that hourly OC measurements are available at SEARCH network sites.

We compared model results against OM measurements at the 4 stations in the SEARCH network that had hourly OM data (BHM, CTR, JST, YRK). The results of the average (JJA) diurnal cycles are shown in the Figure below. It appears that the inclusion of wet deposition of SVOCs has negligible effects on the diurnal cycle. Considering dry deposition of SVOCs slightly reduces the diurnal variability of OM concentrations. Interestingly, the sensitivity studies to access the effect of volatility (LOWVOL, FAST_AGING) lead to a slight shift in overall concentrations, but not to a visible change in the diurnal amplitude of OM concentrations.

The text has been amended in sections 4.1

[...] Our findings show that at the west coast, modeled OC is underestimated in all simulations, while in the Eastern US, both REF and LOWVOL results track observed OC concentrations well during July and August, but underestimate them in June. OC concentrations are overestimated in the FAST_AGING simulation, especially in the Southeast.

We further compared our results to hourly measurements of organic matter (OM) conducted within the Southeastern Aerosol Research and Characterization study (SEARCH, Hansen et al., 2012) to understand the effects of dry and wet deposition of SVOCs on the diurnal cycle of OM. Four stations in the Southeast (North Birmingham, AL - BHM; Centreville, AL - CTR; Yorkville, 270 GA - YRK; Jefferson Street, GA - JST) had measurements available (http://www.atmospheric-research.com/studies/search/SEARCHFactSheet.pdf, last accessed 11 Aug 2014, for site locationsand description). The resulting averaged diurnal cycles are shown in Figure 6. We find that including wet deposition of SVOCs has no effect on the diurnal cycle of OM at these stations, possibly due to the non-local nature of this removal process: washout affects the whole column up to the cloud where the precipitation originates, hence such an event also reduces concentrations aloft which are then advected. Dry deposition instead only acts on the lowest grid cell. Including dry deposition of SVOCs leads to a reduction in the diurnal amplitude of OM concentrations, and a better agreement with observations. In general, modeled diurnal amplitudes are larger than the observed ones. At all stations, with the exception of BHM, observed OM is more or less constant

throughout the day. Judging based on the observations at BHM and minor variations seen at the other stations we observe that the timing of diurnal maxima and minima differ between observations and model. Modeled diurnal cycles indicate a morning minimum in OM concentrations (possibly due to the rise of the boundary layer) and a maximum in the afternoon (maximum of photochemical SOA production), whereas the observed maximum OM concentrations occur in the early morning (around 6 LT) - arguably the time with the lowest boundary layer height and high primary emissions - and the observed minimum is during late afternoon hours (around 18 LT).

In our study we only consider "traditional" SOA formation mechanisms (pure gas-phase oxidation), [...]

and 5.1

[...] This suggests that VBS schemes currently used create a volatility distribution that is too volatile compared to the real atmosphere (observed before by e.g., Grieshop et al., 2009), although other effects may also be important.

Interestingly, when looking at the average diurnal cycles of OM (Figure 6), the effect of changing the volatility distribution leads to a mere shift in concentrations, but not to a change in the diurnal cycle, as it might have been expected.

5.2 Water solubility of SVOCs

And the following figure has been added:

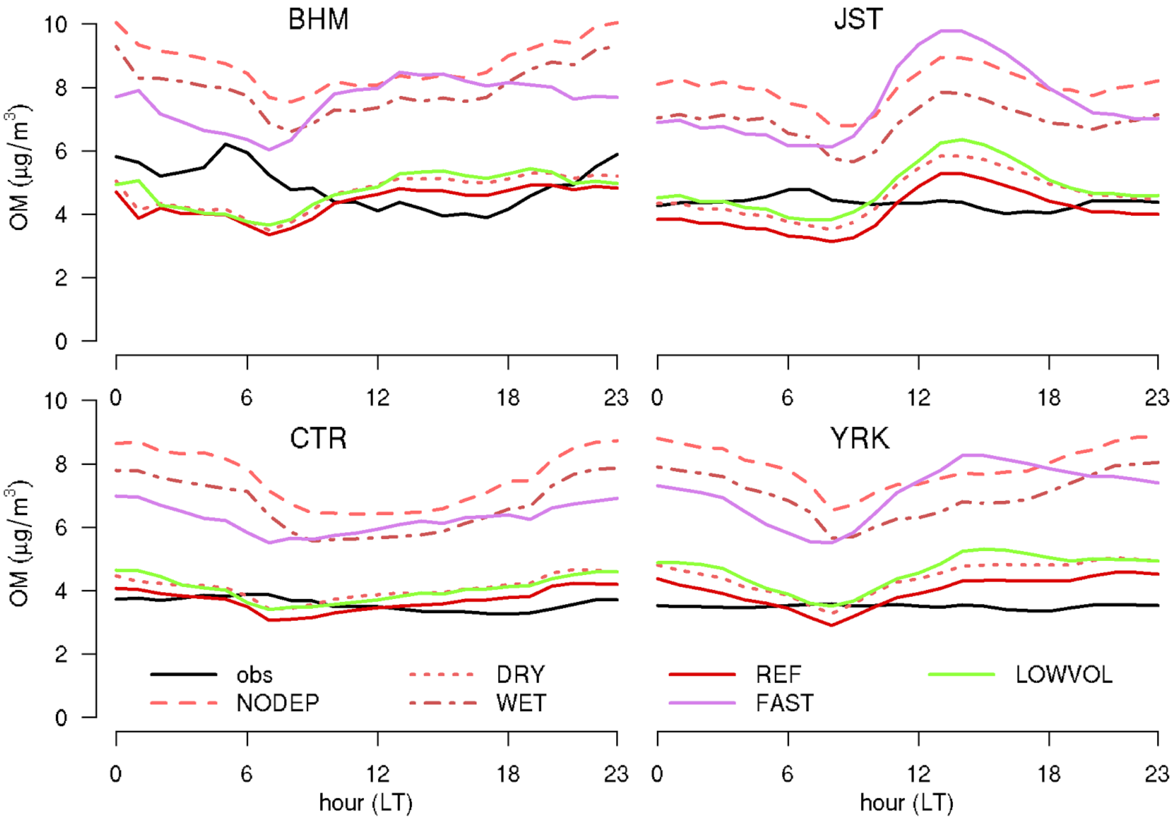


Fig. 6. JJA average diurnal cycles of organic matter (OM) concentrations at 4 field sites of the SEARCH network. Measurements assume an OM/OC ratio of 1.4 (Hansen et al., 2012).

Minor comments:

R1.10 Page 13734, line 25: change "that" to "than"

Changed.

R1.11 Page 13736, line 25: The text references a C bin of 0.001 but Figure 1 represents the lowest volatility bin as 10ˆ-4. Which is it? Please fix either the figure or the text (note that the 0.001 value is stated other places in the text as well, for instance page 13739, line 4).*

It is 10^{-4}, as given in the schematic. The text has been updated accordingly.

R1.12 Page 13738, line 12: Rao et al, 2011 is not the appropriate reference for AQMEII phase 2 emissions inputs since this is an overview article on AQMEII phase 1 and does not include any technical details. Please find a more appropriate reference.

The reference of AQMEII phase 2 has been updated, please refer to our response to R1.2 for detailed changes.

R1.13 Page 13740, line 16: NMB should be -38%, not 0.69.

Corrected.

R1.14 Page 13741, lines 8-10: Why doesn't wet deposition have a greater impact in the southeastern US where both OC concentrations and precipitation are high?

It does have a greater impact in absolute terms, but the relative figures are very similar. We find that wet deposition of condensable organic vapors in general is much less effective than dry deposition (O(10%) vs. O(50%)), probably limited by the amount of liquid water available for partitioning.

R1.15 Page 13742, line 10: The modeled month-to-month evolution may be more similar to the observed evolution but it is still more pronounced than the observed annual pattern.

We agree and have altered the sentence to emphasize that we are discussing the month-to-month evolution:

[...] In the REF simulation with removals, the overall concentrations of OC are underestimated compared to measurements, but the month-to-month evolution is considerably more similar to the observed evolution. [...]

R1.16 Page 13742, line 19-20: This statement is not accurate for wintertime underestimates which are not driven by SOA. The REF and NODEP results look similarly low during wintertime months.

We agree and have rephrased the sentence which now reads:

[...] will be similar. Including these processes would then increase concentrations shown in Fig. 5, predominantly during summer months where SOA contributes most to total OA, potentially closing the gap between

measurements and model results.

R1.17 Page 13744, lines 17-19: Others have also suggested this as well. For instance, Grieshop et al (2009) apply a more aggressive aging scheme (each oxidation step results in C drop of 2 volatility bins rather than 1 and rate constant K_OH = 2x10ˆ-11) to match measured behavior.*

We have included a number of references on this topic:

This suggests that VBS schemes currently used create a volatility distribution that is too volatile compared to ambient aerosols (observed before by e.g., Grieshop et al., 2009; Hodzic et al., 2010; Cappa and Jimenez, 2010; Lee-Taylor et al., 2011), although other effects may also be important.

R1.18 Figure 5: This figure shows some unexpected results in that OC looks unbiased in August but not in other months. This is not what would be expected if SOA under-predictions were driving the model bias for OC. The persistent OC under-prediction in winter months also suggests that SOA/SVOC biases are only one factor in model performance issues for OC. A bit more discussion and interpretations of these results would be useful.

We agree with the reviewer that this is indicates that SOA modeling is not the only factor impacting model performance. We have already addressed the discussion of model performance at several occasions throughout our replies to reviewers (R1.6, R1.7, R1.8, R1.9) and think this sufficiently discusses these comparisons.

R1.19 Figure 8: This is an informative plot. Could the authors make a similar plot for their WRF-Chem results comparing the volatility distributions in different sensitivity runs?

We have created such a plot and included it in the Supplementary Material as Figure S1. It is reproduced below:

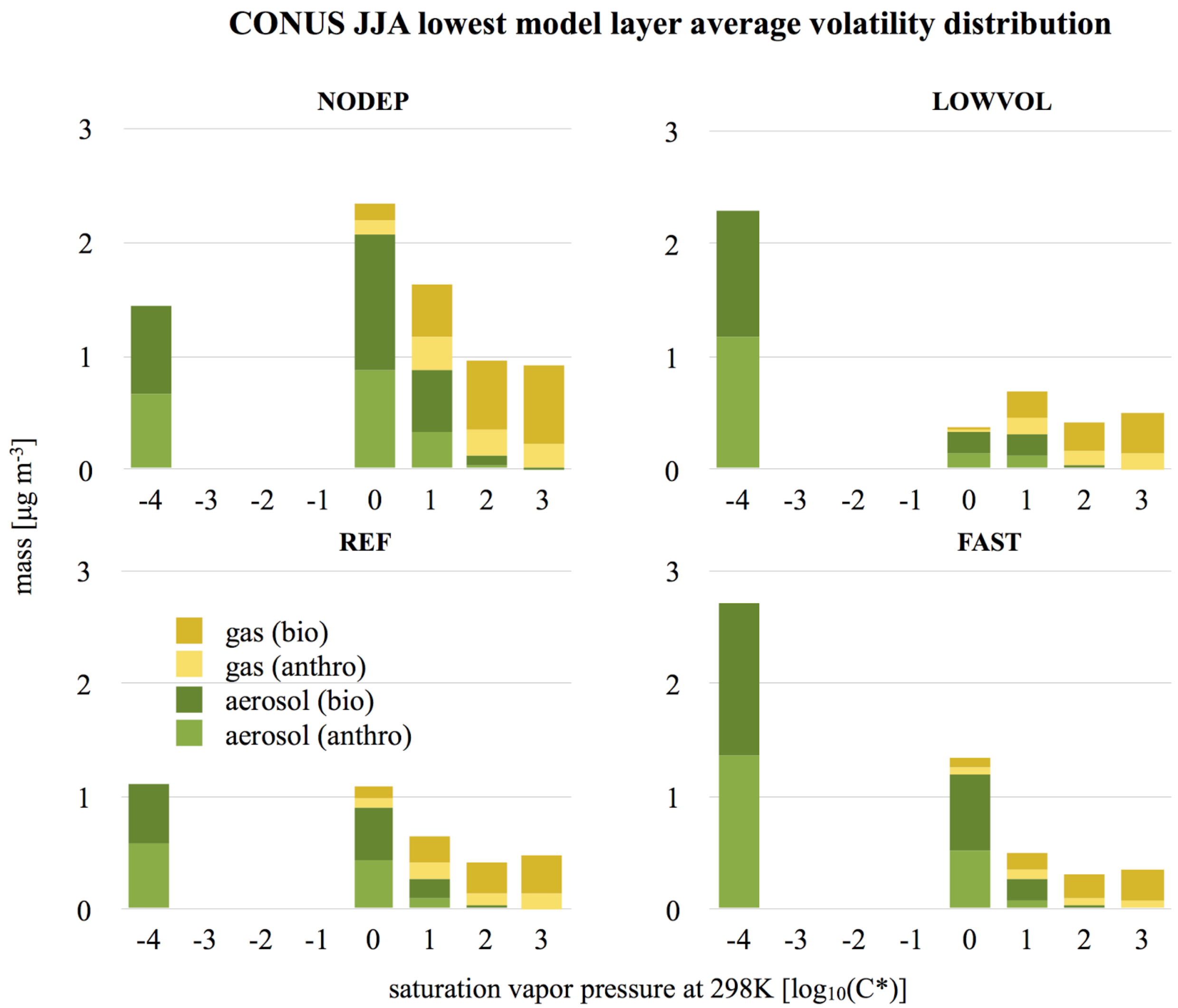


Figure S1. Continental United States, lowest model layer, summer months (June, July, August) average SOA volatility for the case without SVOC deposition (NODEP), the reference case (REF), and the two volatility sensitivity studies (FAST, LOWVOL).

We also reference this figure in the text (section 5.2):

[...] Both changes result in a much less volatile distribution of mass (see also Fig. S1 in the supplementary material) which is less susceptible to gas-phase removals. The reader is referred to the Appendix for a box model study on the effects of these changes. The resulting volatility distributions are comparable to what has been observed in the atmosphere (Cappa and Jimenez, 2010), hence we deem this to be a lower bound of the effect of gas-phase removal on SOA

concentrations. As expected, we find (Table 4) that the efficiency of gas-phase removal is sensitive [...]

Refs: Carleton, A.M., Bhave, P.V., Napelenok, S.L., Edney, E.O., Sarwar, G., Pinder, R.W., Pouliot, G.A., Houyoux, M. (2010) Model representation of secondary organic aerosol in CMAQv4.7, ES&T, 44, 8553-8560.
Grieshop, A.P., Logue, J.M., Donahue, N.M., Robinson, A.L. (2009) Laboratory investigation of photochemical oxidation from wood fires 1: measurement and simulation or organic aerosol evolution, ACP, 9, 1263-1277.

Reproduced tables S1 and S2 from the Supplement

Table S2. Mapping of emitted species as provided in the emissions input (AQMEII phase 2 data, Carbon Bond Mechanism Version 5 (CB05) speciation) onto the MOZART mechanism. Lumped structure species PAR, OLE and IOLE are converted into MOZART lumped molecules species assuming a (mole-wise) fractional contribution of 0.14, 0.02, and 0.84 of C_3H_6, BIGENE and BIGALK (based on measurements by Borbon et al., 2013) and the identities given in the table below.

MOZART species	**Emissions input species (CB05 speciated)**
MACR	ACROLEIN + BUTADIENE13
CH3CHO	ALD2 + ALDX
BENZENE	BENZENE
CH4	CH4
CO	CO
C2H6	ETHA
C2H4	ETH
C2H5OH	ETOH
CH2O	FORM
ISOP	ISOP
CH3OH	MEOH
NH3	NH3
NO2	NO2
NO	NO
HONO	HONO
SO2	SO2
SULF	SULF
C10H16	TERP
TOLUENE	TOL

XYLENE	XYL
C3H6	OLE + PAR
BIGENE	OLE + 2 × PAR, IOLE + 2 × PAR
BIGALK	5 × PAR
C3H8	1.12 × 10^{-2} × CO (Borbon et al., 2013)
CH3COCH3	1.18 × 10^{-2} × CO (Borbon et al., 2013)
MVK	2.40 × 10^{-4} × CO (Borbon et al., 2013)
C2H2	5.87 × 10^{-3} × CO (Borbon et al., 2013)

Table S3. Emissions mapping for aerosol species. Each WRF-chem species listed below is actually 2 variables, for emissions into the Aitken and the accumulation size mode respectively. This is based on a modal aerosol description like e.g. in MADE (Ackermann et al., 1998). We here distribute the emissions input that is not size resolved into the different modes by applying a mass fraction of 0.1 for the Aitken mode and 0.9 for the accumulation mode (based on the work of Elleman and Covert, 2010). Emissions into these two modes are then distributed within WRF-Chem into the size bins of the MOSAIC aerosol module.

WRF-Chem species	**Emissions input species**
PM25	PAL + PCA + PFE + PK + PMFINE + PMG + PMN + PMOTHR + PSI + PTI
NA	PNA
CL	PCL
EC	PEC
ORG	POC
SO4	PSO4
NO3	PNO3

NH4	PNH4
PM_10	PMC

Additional references

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