

Response to Interactive comment by H. O. T. Pye on “Simulating Secondary Organic Aerosol in a Regional Air Quality Model Using the Statistical Oxidation Model: 2. Assessing the Influence of Vapor Wall Losses” by C. D. Cappa et al.

Original comments in **black**. Responses in **blue** and proposed new text is *italicized*.

The Statistical Oxidation Model (SOM) was applied to the South Coast Air Basin (SoCAB) and Eastern US as part of the UCD/CIT regional transport model. The focus was on examining how correcting for vapor wall losses might resolve model/measurement disagreement in terms of SOA magnitude, OC magnitude, and O:C ratios. The SOM model has many nice features, such as the ability to consider wall-loss and fragmentation/functionalization within the chamber fitting procedure as well as explicit predictions of the O:C ratio. The manuscript was well written and easy to follow. My comments are aimed at clarifications.

We thank the commentator for the suggestions as to how to clarify our work. Our responses to specific queries follow below.

Major comments:

1. Make sure that the terms used to characterize simulations as high vs low yield are precisely defined. In this work, high and low refer to the amount of wall loss in the chamber fitting. In Part 1 by Jathar et al., the high and low yield SOM parameterizations refer to low/high NO_x regimes. This is potentially confusing to readers trying to follow the evolution of parameters through the literature.

We will clarify the language used, especially expanding figure and table captions to make clear the distinction. Although we understand the potential for misunderstanding, we note that we do use consistent language within each manuscript, and only use the specific terminology SOM-no, SOM-low, and SOM-high to refer to the effects of vapor wall losses, and not for the influence of NO_x.

2. Table 1: A correlation coefficient (Pearson’s *r*, concordance correlation coefficient, etc) would be useful for model vs. IMPROVE/STN comparisons. Figure S4-S5 look like the correlation between model and obs might be low.

We do not specifically fit a regression line through the data. Nonetheless, we can calculate the concordance correlation coefficient as:

$$\rho_c = \frac{2s_{xy}}{s_x^2 + s_y^2 + (\bar{x} - \bar{y})^2}$$

where \bar{x} and \bar{y} indicate the mean, s_x^2 and s_y^2 are the variance and s_{xy} is the covariance. We will provide these values in an updated Table 1 (shown below). Indeed, in many cases the values are small (close to zero).

Simulation	NO _x parameter ization	Southern California						Eastern US					
		STN ^a			IMPROVE ^b			STN ^a			IMPROVE ^{b,c}		
		Frac. Bias	NMSE	ρ _c	Frac. Bias	NMSE	ρ _c	Frac. Bias	NMSE	ρ _c	Frac. Bias	NMSE	ρ _c
	low	-70	88	0.03	-75	114	0.36	-81	206	0.04	-55	105	0.31
SOM-no	high	-61	69	0.02	-60	85	0.41	-58	166	0.12	-24	84	0.48
	average	-65	78	0.02	-67	97	0.39	-68	180	0.08	-38	89	0.43
	low	-52	64	-0.21	-45	65	0.36	-26	154	0.08	15	85	0.15
SOM-low	high	-39	49	-0.29	-27	47	0.27	-4	171	0.07	38	128	0.10
	average	-45	55	-0.25	-36	54	0.32	-14	160	0.08	28	105	0.12
	low	-25	51	-0.03	-8	46	0.44	26	236	0.15	69	189	0.40
SOM-high	high	-10	38	-0.08	16	43	0.46	45	298	0.15	86	295	0.25
	average	-17	43	-0.05	5	42	0.46	36	265	0.16	79	241	0.31

^a Observed [OA] for STN sites estimated as $1.6([\text{OC}] - 0.5 \mu\text{g m}^{-3})$

^b Observed [OA] for IMPROVE sites estimated as $2.1[\text{OC}]$.

^c Observed [OA] may be biased low by ~25% in the SE US summer due to evaporation after sampling (Kim et al., 2015).

We will amend the text to state:

Error! Reference source not found. lists statistical metrics of fractional bias, normalized mean square error (NMSE) and the concordance correlation coefficients that capture model performance for OA for all simulations for both domains across the STN and IMPROVE monitoring networks. Fractional bias is calculated as:

$$\text{Fractional bias} = \frac{2(C_{OA,sim} - C_{OA,obs})}{C_{OA,sim} + C_{OA,obs}} \quad (1)$$

and the NMSE as

$$\text{NMSE} = \left| \frac{(C_{OA,sim} - C_{OA,obs})^2}{C_{OA,sim} \times C_{OA,obs}} \right| \quad (2)$$

where the subscripts *sim* and *obs* refer to the simulated and observed OA concentrations, respectively. The concordance correlation coefficients (ρ_c) are calculated as:

$$\rho_c = \frac{2s_{sim,obs}}{s_{sim}^2 + s_{obs}^2 + (\overline{C_{OA,sim}} - \overline{C_{OA,obs}})^2}$$

where $\overline{C_{OA,sim}}$ and $\overline{C_{OA,obs}}$ indicate the mean, s_{sim}^2 and s_{obs}^2 are the variance and $s_{sim,obs}$ is the covariance of the simulated and observed OA concentrations.

3. Simulations for 2010 (coinciding with CalNex) and 2013 (coinciding with SOAS/SEAC4RS) would be useful since concentrations have likely evolved significantly since 2005-2006.

Although we certainly agree with Dr. Pye, such simulations are currently outside the scope of this manuscript.

4. Page 30091: How does SOM overcome the issue of dynamic range if it is based on the same chamber data as an Odum 2-product fit? While Figure S2 seems to show the Odum 2-product fits have some serious errors at lower delta(HC), are those lower delta(HC) constrained by the experimental data?

The “dynamic range” issues arise from the limited number of parameters in the 2-product model, not the data. The SOM overcomes this issue by using a greater number of parameters that span a wider, more continuous volatility range. That said, one can certainly ask the question how well the SOM (or any model) will do at very low concentrations where the measurements are at their limit. Here, we rely on the

structure of the SOM itself, in that the SOM is developed to use a self-consistent set of physically-based rules to describe the chemical evolution of the system. This physical basis to the model provides for greater flexibility and performance at low concentrations (and over a larger dynamic range in general) compared to the 2-product model. We note here also that unpublished comparisons with the GECKO-A model of SOA formation, which is a chemically-explicit model, indicate generally good correspondence between the two models. We will modify the text to read:

We have determined that this lack of robustness is a result of the limited dynamic range of the 2-product model. *This can be contrasted with the SOM, which includes many more species that span a wider, more continuous volatility range, making it more flexible when fitting the laboratory data.*

5. Page 30095: Is the high or low NO_x regime more sensitive to wall-loss corrections? A column could be added to table S1 indicating the SOA yield (for a given set of conditions like total OA, etc.) relative to the uncorrected yield. What if instead of averaging the high/low NO_x regime results, the authors only looked at high or low-NO_x results? This would allow readers to infer their own SOA enhancements based on the relative dominance of the pathways. It appears that the low-NO_x regime may be more sensitive to the wall-loss correction. In SoCAB, the high-NO_x pathway is likely to be more relevant. Thus, figure 1 may overestimate the potential impact of wall-loss correction.

Dr. Pye raises an interesting point. How do the R_{wall} values differ between the low-NO_x and high-NO_x simulations? To test this, we have plotted a subset of the R_{wall} values simulated for the eastern US but where the R_{wall} values were not calculated as the ratio between the averaged SOM-high or SOM-low and the SOM-no simulations, but where we have calculated this for each of the NO_x parameterizations individually. (The specific subset selected here corresponds to the data shown in Figure S5 that were compared with the eastern US observations and was chosen because these simulation results were already extracted from the model runs. Given the large number of sites located across the eastern US, and thus corresponding to a wide range of absolute values and conditions, we fully expect that if all of the data from the individual runs were considered, as was done in Fig. 3, similar conclusions would be reached.) Since, as the authors note, the terminology can get confusing, we specifically calculated:

$$R_{wall}(low\ NO_x\ parameterization) = \frac{[SOA]_{lowVWL,lowNO_x}}{[SOA]_{noVWL,lowNO_x}}\ or = \frac{[SOA]_{highVWL,lowNO_x}}{[SOA]_{noVWL,lowNO_x}}$$

and

$$R_{wall}(high\ NO_x\ parameterization) = \frac{[SOA]_{lowVWL,highNO_x}}{[SOA]_{noVWL,highNO_x}}\ or = \frac{[SOA]_{highVWL,highNO_x}}{[SOA]_{noVWL,highNO_x}}$$

and where the subscript "VWL" indicates the vapor wall loss condition and the subscript "NO_x" indicates the NO_x condition. This can be contrasted with what was done in the manuscript, which was:

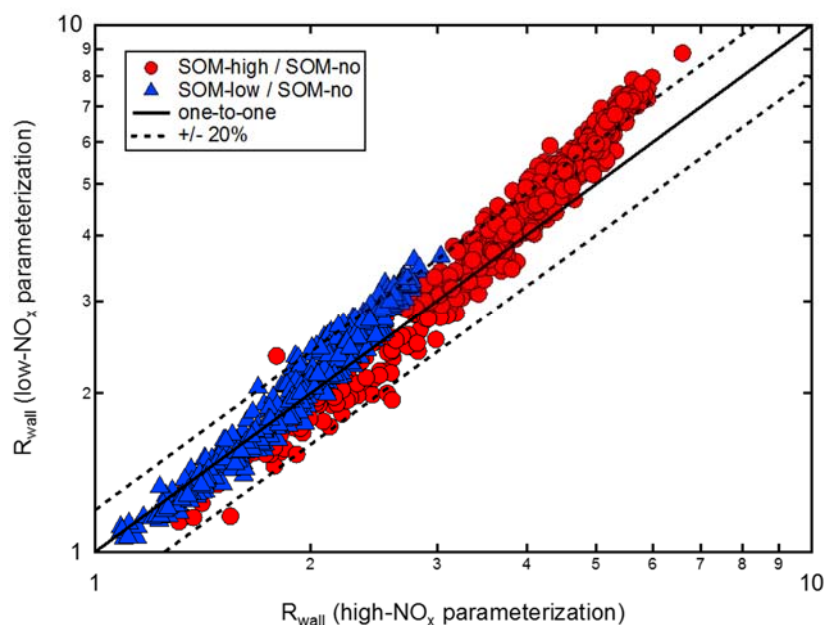
$$R_{wall}(lowVWL) = \frac{[SOA]_{lowVWL,lowNO_x} + [SOA]_{lowVWL,highNO_x}}{[SOA]_{noVWL,lowNO_x} + [SOA]_{noVWL,highNO_x}}$$

or

$$R_{wall}(highVWL) = \frac{[SOA]_{highVWL,lowNO_x} + [SOA]_{highVWL,highNO_x}}{[SOA]_{noVWL,lowNO_x} + [SOA]_{noVWL,highNO_x}}$$

and where we have again explicitly used “VWL” to indicate the vapor wall loss condition (low or high). It is clear that there is some difference between the simulated R_{wall} values between the low- NO_x and high- NO_x parameterizations, although most points fall close to the one-to-one line. At very low R_{wall} values, the high- NO_x parameterization gives slightly lower R_{wall} than does the low- NO_x parameterization for both the SOM-lowVWL and SOM-highVWL cases. But as the absolute R_{wall} values increase the opposite is true. Regardless, the differences between the NO_x -parameterizations are much smaller than the absolute values of the simulated R_{wall} values. We intend to include this comparison in the revised manuscript, with the figure below added to the supplemental material (along with the equations above) and the following sentence added at P30095, Line 19:

If R_{wall} values are calculated using the simulated SOA concentrations from either the low- NO_x or high- NO_x parameterizations individually, as opposed to the average values used above, very similar results are obtained (Figure SX).



Minor comments:

- Page 30085, line 10-11: Briefly recap how vapor pressure affects wall loss (decreasing vapor pressure leads to increasing losses?)

We will modify the sentence to read:

Recent observations have demonstrated that organic vapors can be lost to Teflon chamber walls, and that the extent of loss is related to the compound vapor pressures *with lower vapor pressure compounds partitioning more strongly to the walls than higher vapor pressure compounds* (Matsunaga and Ziemann, 2010; Kokkola et al., 2014; Krechmer et al., 2015; Yeh and Ziemann, 2015; Zhang et al., 2015).

- Page 30088, line 20: Should k_{wall} and α_{wall} also be mentioned as tunable?

Although these are not tuned in the model here, they are theoretically tunable. However, one should recognize these are coupled, as discussed in Zhang et al. (2014) and shown in their Fig. S4. For the current

study, rather than explicitly tuning k_{wall} (and α_{wall}), we instead consider two specific values of k_{wall} . The reason for this decision is discussed on Page 30089, Section 2.3. To clarify this, we will modify Section 2.3 to state:

It should be noted that the influence of vapor wall losses is inherent in the fit parameters, and in the absence of walls (i.e. in the atmosphere) the predicted SOA formed will be larger when the fits account for vapor wall losses. *A base case set of parameters with no vapor wall losses assumed during fitting (termed SOM-no) was determined using $k_{\text{wall}} = 0$. In Zhang et al. (2014), an optimal value of $k_{\text{wall}} = 2 \times 10^{-4} \text{ s}^{-1}$ was determined for the California Institute of Technology chamber based on simultaneous fitting of the SOM to a set of toluene photooxidation experiments conducted at different seed particle concentrations. Unlike in Zhang et al. (2014), the values of k_{wall} used here were not determined during model fitting. This is because the absolute value of k_{wall} is not well constrained by a single experiment, and the simulations require vapor wall loss corrected parameters for VOCs besides toluene. Therefore, two specific bounding cases that account for vapor wall loss are instead considered based on the results from Zhang et al. (2014). Specifically, values of $k_{\text{wall}} = 1 \times 10^{-4} \text{ s}^{-1}$ and $2.5 \times 10^{-4} \text{ s}^{-1}$ are considered, corresponding to a low vapor wall loss case (SOM-low) and high vapor wall loss case (SOM-high), respectively.*

8. Page 30090, line 6: In which direction is the correction conservative? High or low wall loss?

The question is in reference to the selected value of α_{particle} used in the model, here $\alpha_{\text{particle}} = 1$. We have shown previously (Zhang et al., 2014) that the influence of vapor wall losses is increased when the assumed value of α_{particle} is decreased. Thus, the correction (or really, assumption of $\alpha_{\text{particle}} = 1$) is “conservative” in that it minimizes the influence of vapor wall losses. This is true for both the high and low vapor wall loss cases. But, of course, the use of the larger assumed k_{wall} (i.e. “high” vapor wall loss case) is less conservative than the use of the smaller assumed k_{wall} (i.e. the “low” vapor wall loss case). We will modify the sentence to be:

Thus, a conservative estimate *that minimizes* the influence of vapor wall losses on SOA formation is obtained using $\alpha_{\text{particle}} \geq 0.1$.

9. Page 30092, line 27: May want to mention that the CMAQ POA treatment by Simon and Bhawe, although non-volatile, does account for aging of POA along a -1 van Krevelen slope due to OH reaction such that O:C evolves in that atmosphere (with a distinct diurnal profile).

We thank Dr. Pye for pointing out this reference. However, as at this point in the manuscript we are discussing the operation of the SOM model specifically, it does not seem the appropriate location to mention the Simon and Bhawe study. It would seem that the addition of such a reference around Page 30103, Line 9/10 would be more appropriate. We will add a reference, in addition to the Murphy et al. (2011) reference.

10. Page 30094, line 1-4: While not always perfectly simulated, we do have some confidence in the ability of models to predict NO:HO₂ branching. Models (at fine resolution, perhaps not at 36 km) capture spatial distributions in branching and GEOS-Chem captures seasonal trends in high vs. low-NO_x isoprene oxidation products (Kim et al. 2015 ACP). I’m not sure if Carlton et al. 2010 is a good reference here.

We assume that Dr. Pye is referring specifically to the paper “Sources, seasonality, and trends of southeast US aerosol: an integrated analysis of surface, aircraft, and satellite observations with the GEOS-Chem chemical transport model” by Kim et al. (2015), as there is more than one paper in ACP by Kim et al. in

2015. It does not appear that that paper specifically presents NO:HO₂ ratios or compares the simulated NO:HO₂ to observed values. The paper does state “Aerosol chemistry is coupled to HO_x -NO_x -VOC-O₃-BrO_x tropospheric chemistry with recent updates to the isoprene oxidation mechanism as described by Mao et al. (2013),” but this does not seem to be a demonstration that the branching is correct. Further, the SOA from isoprene in this paper is “produced with a yield of 3%...formed at the point of emission,” and that while they “use four separate tracers in the model to track SOA formed from isoprene and monoterpenes via the high- and low-NO pathways” they also note that “This tracer separation is purely diagnostic as the SOA yields are assumed here to be the same in both pathways”. This is not to say that the overall variability in spatial distributions and seasonal trends in branching between low-NO_x and high-NO_x pathways are not well simulated, but it would be great if Dr. Pye were able to point us towards a reference that more directly addresses this issue (or let us know if we are looking at the wrong reference).

11. Page 30096, line 1: This line reads that there is more absolute SOA over the ocean than land. Is that what was intended?

No, this is not what was intended. This was stated backwards. It should instead read: “Indeed, the ratio between the predicted average SOA *in downtown LA (urban)* to that over the Pacific Ocean near the coast of LA (*regional*) and decreases from 2.3 (SOM-no) to 1.5 (SOM-low) to 1.3 (SOM-high), for example.” We thank Dr. Pye for catching this error.

12. Page 30096, line 17-18, the authors may want to restrict the fSOA enhancements here to values from the Riverside or LA-Basin locations as higher ratios correspond to low absolute OA values.

We appreciate the suggestion and will add more specific values during revision. Inspection of Fig. 3 indicates that the SOM-no, SOM-low and SOM-high f_{SOA} values in Riverside are ~0.2, ~0.35 and 0.5, respectively.

13. Page 30099, was there an overall model bias in CO?

Yes, it would appear that the simulated CO is biased slightly high. As stated, the simulated background [CO] = 130 ppb while the observed background [CO] ~ 105 ppb.

14. Page 30100: Keep in mind that NO_x has changed significantly from 2005-2013 (e.g. Russell et al. 2012 ACP) and that would affect the IEPOX-OA abundance. Changes in sulfate/acidity would also affect IEPOX-OA (e.g. Pye et al. 2013, Marais et al. 2015 ACPD).

We thank Dr. Pye for pointing these issues out. We will revise the manuscript to note these points in the context of the model/measurement comparison across years. Specifically, we intend to add the sentence:

Additionally, it should be kept in mind that the ambient NO_x concentrations in SoCAB have decreased substantially from 2005-2013 (Russell et al., 2012).

15. Page 30102: The fraction fossil discussion that compares 2005 simulations to 2010 field data may need more caveats in its current form (ie highlighting potential changes in fossil fraction from 2005 to 2013). Could the authors not estimate the fraction fossil of SOC in the model given that the O:C ratio is known for the model species? That may eliminate some of the discrepancy in comparison.

Dr. Pye raises a good point, that the carbon mass can be estimated from the SOA mass and the species-specific O:C values, which can then be used to calculate a carbon-specific fossil fraction. Specifically, the mass concentration of carbon (C_c) is related to the mass concentration of SOA (C_{SOA}) as:

$$C_c = \frac{C_{SOA}}{O:C + 1}$$

We have used the above equation to calculate C_C values for each SOA type, and from this the carbon-specific fossil fractions (F_{SOC}). We find that the calculated fossil fractions generally change by a small amount. In some cases the carbon-specific fossil fraction is larger than the SOA fossil fraction and in others it is smaller. The average absolute difference for SoCAB is 0.00 and for the eastern US is 0.02. The calculated F_{SOA} and F_{SOC} values for the low- and high- NO_x simulations for the three vapor wall loss cases (SOM-no, SOM-low and SOM-high) are compared in the table below. We will add this table to the supplemental material and include the following in the main text on Page 30102:

The fossil fraction of secondary organic carbon can be calculated from the simulated SOA concentrations by accounting for the differences in the O:C atomic ratios of the different SOA types to facilitate more direct comparison between the simulations and observations. Specifically, the carbon mass concentration (C_C) is related to the SOA mass concentration (C_{SOA}) for a given SOA type through the relationship:

$$C_C = \frac{C_{SOA}}{O:C+1} \quad (1)$$

The O:C values of the different SOA types are not constant in the SOM due to the continuous evolution of the product distribution. However, for a given SOA type the simulated O:C values vary over a narrow range (Cappa et al., 2013) and thus an average value can be used. The resulting $F_{SOC,fossil}$ values are compared with the $F_{SOA,fossil}$ values in Table S2 and are found to be very similar.

Vapor Wall Loss Case	NO_x condition	Central LA		Riverside	
		SOA	SOC	SOA	SOC
SOM-no	high- NO_x	0.27	0.25	0.28	0.25
	low- NO_x	0.44	0.41	0.40	0.37
SOM-low	high- NO_x	0.22	0.23	0.27	0.28
	low- NO_x	0.32	0.30	0.35	0.33
SOM-high	high- NO_x	0.22	0.25	0.28	0.31
	low- NO_x	0.33	0.32	0.37	0.36
		Atlanta		Smokey Mountains	
		SOA	SOC	SOA	SOC
SOM-no	high- NO_x	0.10	0.08	0.14	0.12
	low- NO_x	0.17	0.15	0.15	0.13
SOM-low	high- NO_x	0.19	0.18	0.27	0.27
	low- NO_x	0.18	0.17	0.22	0.21
SOM-high	high- NO_x	0.25	0.27	0.32	0.35
	low- NO_x	0.20	0.19	0.24	0.23

16. Table S1 seems to indicate monoterpenes and sesquiterpenes have the same SOA yield. Why was that decision made?

The values in Table S1 do not indicate that the monoterpenes and sesquiterpenes have the same SOA yields. We assume that the SOM parameters that describe the SOA formation are the same. The sesquiterpenes have a greater number of carbon atoms than the monoterpenes. Consequently, the sesquiterpenes have a larger SOA yield than the monoterpenes because the oxidation products from sesquiterpene oxidation have lower volatility. We will clarify this aspect by adding the following to Table S1:

**Although the same set of parameters are used to describe the formation of oxidation products and SOA from monoterpenes and sesquiterpenes, the SOA yield from sesquiterpenes is larger than for monoterpenes due to the larger number of carbon atoms comprising sesquiterpenes.*

17. What oxidants (OH, O₃, NO₃?) are considered for SOA purposes?

In the SOM we consider reactions with OH, O₃ and NO₃, although make particular simplifications for computational efficiency. In particular, each precursor VOC is allowed to react with either OH, O₃ or NO₃ as characterized by an oxidant-specific rate coefficient. However, the products and product distributions of the first-generation products are assumed to be oxidant independent. This simplification is identical to that employed in CMAQv4.7 (Carlton et al., 2010). Reactions of subsequent oxidized SOM products then occur only via reaction with OH radicals according to the SOM parameterization associated with that precursor VOC (as determined by fitting photooxidation experiments). Reactions with O₃ and NO₃ will be most important for the mono- and sesquiterpenes. We will add the following information in the section 3.5 Model Simulations and Outputs:

Each precursor VOC is allowed to react with either OH, O₃ or NO₃ as characterized by an oxidant-specific rate coefficient, although the products and product distributions of the first-generation products are assumed to be oxidant independent. This simplification is identical to that employed in CMAQv4.7 (Carlton et al., 2010). Reactions of subsequent oxidized SOM products then occur only via reaction with OH radicals according to the SOM parameterization associated with that precursor VOC (as determined by fitting the photooxidation experiments).

18. Figure 5: I'm surprised the base (SOM-no) simulation gets such high OA/CO ratios. In our CMAQ and CMAQ-VBS simulations (Woody et al. 20105 ACPD), we see slopes of 8 and 66 ug/m³/ppm compared to 108 in the observations for SOA/del(CO) vs. log(NO_x/NO_y).

The reported OA/ Δ CO ratio for the SOM-no simulation was 23 $\mu\text{g m}^{-3} \text{ppm}^{-1}$. Certainly this is larger than the 8 $\mu\text{g m}^{-3} \text{ppm}^{-1}$ reported by Woody et al. for their standard CMAQ simulation, but it is lower than the 66 $\mu\text{g m}^{-3} \text{ppm}^{-1}$ reported for their CMAQ-VBS simulation. It is difficult to intuit the reason for this difference between models. It is possible that it arises from the difference in datasets used to develop the SOM parameterization as compared to the 2-product and VBS parameterizations used in Woody et al. (2015), although we note that the results in Jathar et al. (2015b) (which focus on the performance of SOM-no compared to other model formulations) suggest that minimal differences between simulations should be obtained due to this difference. It is possible that the difference is due to the different simulation periods and specific locations, although this seems relatively unlikely. Although establishing the exact reason for such a difference in the base model performance would certainly be of interest, it is outside of the scope of the current study.

19. Provide an estimate of the amount of computer processing time required for a SOM vs. base simulation.

To quote from Jathar et al. (2015a),

All simulations were performed for both domains: SoCAB and the eastern US. The simulations were performed on a computer cluster operated and maintained at the University of California, Davis. Each simulation was performed using Intel Core i5-3570s for a total of 40 core processors and shared memory of 40 GB. The simulations were performed for 19 days with the first 5 days used for spin up. For the SoCAB, each simulated day required approximately 4 h of elapsed time so a 19-day episode was simulated in less than 4 days. For the eastern US, each simulated day required approximately 9 h of elapsed time so a 19-day episode was simulated in about 8 days.

These numbers can be compared with simulations run using the 2-product “Base” model in Jathar et al. (2015b). These “Base” simulations took on average about 30 hours for a 19 day episode in the SoCAB, or 1.6 h per day, so ran faster by a factor of 2.5. However, the base model was run using 16 size sections as compared to the 8 used with the SOM, and thus the actual difference was smaller most likely by somewhere around a factor of 2. We will add the following sentence at the end of Section 3.2:

The use of the SOM to represent SOA formation leads to an increase of about a factor of 2.5 or less in computer processing time required compared to use of the 2-product model.

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