Response to Reviewer #2

Reviewer #2 brings up several important issues that we have now addressed and clarified. Our specific responses can be found below, with reviewer comments in black and our responses in blue.

The authors present measurements of loss rates of oxidized vapors within Teflon chambers. These vapors are produced from photooxidation of high volatility volatile organic compounds on timescales ranging from 1 hr to 7 hrs. After formation, photoxidation was stopped, and the decay of different compounds was monitored using CIMS. After 12 hrs the temperature of the chamber was increased to induced evaporation of the vapors from the walls. These observations were interpreted to deduce values for the effective absorbing wall mass concentration (Cw) and the accommodation coefficient associated with wall deposition of the vapors. The authors find a relationship between Cw and the compound vapor pressure. They also find a relationship between the accommodation coefficient and the compound vapor pressure. They conclude that loss of vapors to chamber walls may be compound specific and more important for lower volatility compounds that apparently are transferred more rapidly to the walls due to their larger accommodation coefficients. Overall, this is a very interesting and important study. Since I can see this serving as the basis of many future studies and playing a key role in the interpretation of future chamber SOA studies, I think that it is critical that it be as clear as possible, and also fully consider any potential artifacts. My comments are made with this in mind. There are certainly times where more information could be provided to help the reader fully understand what was done. Most importantly, the authors need to consider the implications of vapor deposition during the photooxidation stage, the potential influence of interferences in the CIMS, and the potential influence of (or corrections for) "background" signals in the CIMS. How might any of these influence the results, especially the relationships between Cw and accommodation coefficients with vapor pressure? Specific comments and suggestions are provided below.

P26768/9: The authors might note that microscopic reversibility would suggest that the accommodation coefficient for uptake will be equal to that for desorption, which together influence the time it takes to establish equilibrium. Regarding Eqn. 1 and 2, does this formulation imply that the concentration of "vapor i that has accumulated on the chamber wall" is in units of per volume of air?

1) Yes, we have added further discussion regarding the meaning of accommodation coefficient in Section 6, also given below:

"*The significance of* $\alpha_{w,i}$ *is twofold: first, the accommodation coefficient for the desorption of organic molecules from the gas-wall interface equals that for the adsorption/uptake process, which together influence the time needed to establish equilibrium; and second, diffusion in the chamber wall is not considered in the theoretical framework and consequently, the best-fit* $\alpha_{w,i}$ *will reflect the mass transfer resistance in both the gas-wall interface and the chamber wall layer*".

2) Yes, the concentration of vapor *i* in the chamber walls is in the units of g m^{-3}. We have added an Appendix to the manuscript listing all the quantities and corresponding units, also shown below:

A (m^2)*: Total surface area of the chamber wall*
$\alpha_{p,i}$ *(dimensionless): Accommodation coefficient of organic vapor i on particles*
$\alpha_{w,i}$ *(dimensionless): Accommodation coefficient of organic vapor i on the chamber wall*
$C_{0,i}$ (g m^{-3})*: Concentration of organic vapor i over the gas-wall interface*
C_i^* (g m^{-3})*: Saturation concentration of organic vapor i*
$\overline{C}_{tot,i}$ (g m^{-3})*: Total concentration of organic vapor i in the chamber*
$\overline{C}_{v,i}$ (g m^{-3})*: Concentration of organic vapor i in the well-mixed core of the chamber*
$C_{v,i}$ (g m^{-3})*: Local concentration of organic vapor i in the boundary layer adjacent to the wall*
$\overline{C}_{w,i}$ (g m^{-3})*: Concentration of organic vapor i that has accumulated on the chamber wall*
C_w (g m^{-3})*: Equivalent mass of absorbing organic material on the chamber wall*
$\overline{D}_p$ (m)*: Number mean particle diameter*
$\mathcal{D}_e$ (m^2 s^{-1})*: Eddy diffusivity*
$\mathcal{D}_i$ (m^2 s^{-1})*: Molecular diffusivity*
δ (m)*: Thickness of the boundary layer adjacent to the wall*

H_i (dimensionless): Henry's law constant of organic compound i

$J_{v,i}$ ($g\ m^{-2}\ s^{-1}$): Vapor flux arriving at the gas-wall interface

$J_{w,i}$ ($g\ m^{-2}\ s^{-1}$): Vapor flux evaporating from the wall

K_e (s^{-1}): Eddy diffusion coefficient

$K_{w,i}$ ($m^3\ g^{-1}$): Gas-wall partitioning coefficient

$k_{w,depo,i}$ (s^{-1}): Deposition rate coefficient to the wall

$k_{w,evap,i}$ (s^{-1}): Evaporation rate coefficient from the wall

$\overline{M_w}$ ($g\ mol^{-1}$): Average molecular weight of the absorbing organic material on the wall

N_p (m^{-3}): Total number concentration of suspended particles

$p^0_{L,i}$ (atm): Vapor pressure of organic compound i as a liquid

γ_i (dimensionless): Activity coefficient in the wall layer on a mole fraction basis

$\bar{v}_i$ ($m\ s^{-1}$): Mean thermal speed

V (m^3): Total volume of the chamber

Figure 2 and P26775: One aspect unclear from this figure is whether the signals were corrected for "background." For some of the compounds, the first point in the time series is close to zero, while for many others it is well above zero. Related to this, for some of the compounds the signal at the end of the experiment is lower than that in the very first data point. It is unclear, as presented, what this means or how it can be interpreted. Is this a decrease below the initial background? One example where this really stands out is in the bottom left-hand panel of the first page of Fig. 2 (26795). The signal of this species (m/z = 241) is relatively constant for a while before shooting up during the photooxidation phase. But by the end of the study the signal has decreased below that initial stable period. Clarification of exactly how the data are being presented with respect to whether a background subtraction has been performed or not is needed. The authors make no mention of the potential for interferences in the CIMS measurements. More specifically, of detection of two different compounds with the same m/z but different vapor pressures. What is the resolution of the CIMS? Can different compounds with the same nominal m/z be distinguished? What would be the implications if there were two compounds at one m/z, one that decays fast and one that decays slow? Can this be ruled out?

1) The time resolution of the CIMS employed in this study is ~ 9 min. The lights on time during each experiment might occur right in the middle of one CIMS measurement cycle. This is why for certain species shown in Figure 2, the starting concentration is even higher than the final concentration after ~ 15 h of dark decay. We have redrawn this figure in the revised manuscript, including 60 min of chamber air sampling period (background) before lights on.

Prior to the start of each experiment, the purified air in the chamber is sampled, and this is subtracted off as the CIMS background signal. The background signal is fairly consistent between the masses and over time. The signals are then normalized by the overall intensities of H_2O_2 and H_2O to ensure a steady supply of the reagent ion (CF_3O^-). We have added the background subtraction description in Section 3.

2) The CIMS employed in this study has unit mass resolution, which means species sharing the same molecular weight might be detected with the same m/z ($[R\cdot CF_3O]^-$ or $[X_{[H]}\cdot HF]^-$). Because of this, we are particularly careful in selecting oxidized organic vapors from each VOC+OH system. For the isoprene+OH, α-pinene+OH, and dodecane+OH systems, organic compounds selected were all identified in our previous studies with proposed mechanisms for their formation and removal pathways. The simulated temporal profiles of individual compounds match well with observations (Paulot et al., ACP, 2009; Yee et al., JPCA, 2012; Zhang et al., ACP, 2014). For the toluene+OH system, we selected only three ions and assigned structures proposed by MCMv3.2 to them. MCMv3.2 simulations of these three compounds match well with the CIMS observed time-dependent profiles. Considering that the previously proposed mechanisms for each compound can explain the CIMS observations very well, it is unlikely that the chance that several products share the same m/z in the current study. However, since we cannot absolutely rule out the possibility, we estimate uncertainties here as a result of the failure to distinguish two compounds with the same nominal m/z. Consider two organic molecules A and B, with formulas of $C_xH_yO_z$ and $C_{x+1}H_{y+4}O_{z-1}$, respectively. According to relationships between the vapor pressure and elemental composition that have been used in the literature (e.g., Donahue et al., 2011; Cappa and

Wilson, 2012), addition of one O atom would lead to a decrease of the logarithm of vapor pressure by 0.6 – 2.2 atm, depending on the actual functionality. Addition of one C atom would in general lead to a decrease of logarithm of vapor pressure by ~ 0.5 atm. As a result, the vapor pressure of molecule B can be up to ~ two orders of magnitude higher than that of molecule A, and accordingly, the wall deposition rate of molecule A would be a factor of ~ 3-5 higher than that of molecule B.

P26755: Where the authors note: "When the chamber temperature was increased from 25 to 45 C, with all the other experimental conditions held constant, the concentrations of most compounds in the chamber increased: : :" they might consider noting that the increase in many cases was relatively minor relative to the initial peak signal.

Yes, we have added a comment on this.

"*When the chamber temperature was increased from 25 ℃ to 45 ℃, with all the other experimental conditions held constant, the concentrations of most compounds in the chamber increased to a minor degree relative to the initial peak signal, reflecting modest desorption of vapors from the chamber wall*".

Eqns. 12 and 13, and subsequent discussion: Here the authors assume that the total amount of species i can be estimated from the "initial" concentration of vapor, which (although not explicitly stated) I assume to be the concentration (CIMS signal) at the point where the lights are turned off. One point raised by Paul Ziemann in his comment is the extent to which vapor wall deposition during the photooxidation/product generation stage might influence the results. Vapor wall deposition during the formation stage would tend to decrease the Ctot,i values, as estimated from the CIMS vapor measurements. This would have the effect of decreasing the numerators, which would in turn decrease the estimate of Cw. To the extent that the (potential) Ctot,i underestimate correlates with vapor pressure, the Cw estimates might then evidence an apparent vapor pressure dependence, as was observed. I think that this possibility needs to be considered, as well as the subsequent consequences for the Henry's Law interpretation. Additionally, as it is unclear whether the data have been "background" corrected or not, this also needs to be addressed, as offsets due to different species (potentially) having different backgrounds would lead to disparate results. This latter point can be easily dealt with by clarifying the data presentation.

We did not use the the concentration (CIMS signal) at the point at which the lights are turned off as the total organic concentration ($\overline{C}_{\mathrm{tot,i}}$). As shown in Eqs (16) and (17) in the revised manuscript (also given below), $\overline{C}_{\mathrm{v,i@298K}}$ and $\overline{C}_{\mathrm{v,i@318K}}$ can be measured by CIMS. $K_{\mathrm{w,i\ @298K}}$ and $K_{\mathrm{w,i\ @318K}}$ can be calculated by Eq (14). Two unknown parameters remain, i.e., $\overline{C}_{\mathrm{tot,i}}$ and C_{w}. Here we combine Eqs (16) and (17) and solve them as a equation set so that the calculated $\overline{C}_{\mathrm{tot,i}}$ value is actually the total concentration of organic vapor *i* generated during the photooxidation period. Therefore, we believe there are no significant uncertainties in this calculation.

$$\frac{\overline{C}_{\mathrm{w,i@298K}}}{\overline{C}_{\mathrm{v,i@298K}}} = \frac{\overline{C}_{\mathrm{tot,i}} - \overline{C}_{\mathrm{v,i@298K}}}{\overline{C}_{\mathrm{v,i@298K}}} = K_{\mathrm{w,i\ @298K}} C_{\mathrm{w}} \tag{16}$$

$$\frac{\overline{C}_{\mathrm{w,i@318K}}}{\overline{C}_{\mathrm{v,i@318K}}} = \frac{\overline{C}_{\mathrm{tot,i}} - \overline{C}_{\mathrm{v,i@318K}}}{\overline{C}_{\mathrm{v,i@318K}}} = K_{\mathrm{w,i\ @318K}} C_{\mathrm{w}} \tag{17}$$

We have revised the paragraph regarding the calculation of C_{w}:

"*Ideally, C_w can be obtained if the initial total concentration ($\overline{C}_{tot,i}$) and equilibrium gas-phase concentration ($\overline{C}_{v,i}$) of vapor i can be measured by CIMS. However, since the fraction of organic compound i in the chamber walls at the onset of vapor wall deposition is unknown, we estimate C_w via the combination of equilibrium partitioning expressions at two different temperatures, e.g., 298 and 318 K…*".

"*…In this manner, both $\overline{C}_{tot,i}$ and C_w can be calculated by solving the equation set (16) and (17)*".

Eqns. 12/13: More details are required at this point in the manuscript regarding the calculation of the species-specific and T-dependent Kw values. The figure caption indicates that the EVAPORATION model is used to estimate compound vapor pressures, but this information should be in the main text. Further, it is not clear what assumption was made regarding the value for gamma, the activity coefficient, or for the assumed molecular weight of the absorbing material, both of which seem to be required in Eqn. 9

to allow for calculation of Kw.

Yes. We have added these details in the revised manuscript, as shown as below:

"*where* $p^0_{L,i}$ *is the vapor pressure of compound i as a liquid. We calculate* $p^0_{L,i}$ *by the average of two group contribution methods, 'SIMPOL.1' developed by Pankow and Asher (2008) and 'EVAPORATION' developed by Compernolle et al. (2011).* γ_i*, the activity coefficient in the wall layer on a mole fraction basis, is assumed to be unity in this study, R is the gas constant, T is temperature, and* $\overline{M_w}$ *is the average molecular weight of the absorbing organic material on the wall, which is assumed to be 250 g mol*$^{-1}$".

It is also not clear exactly how the information at the two temperatures is used? Are the reported values averages from the two temperatures? Are both reported? Only in the Table 2 caption is it stated that Cw is calculated from the "combination" of the two equations. Is this an average? Are the reported uncertainties from a standard deviation of the two measurements, or some other uncertainty estimate? Do the Cw values from the two temperatures typically agree well? It might also be useful to add the enthalpies of vaporization (which control the T-depedence of the vapor pressure) to Table 2 for reference.

As we explained above, only one C_w value is obtained from calculation combining Eqs (16) and (17) as a equation set because there is another unknown parameter $\overline{C}_{tot,i}$. By doing this, uncertainties for the total amount of vapor *i* in both gas and wall phases are minimized.

Fig. 3: It appears that 30 min average data are only used for one of the data sets. The caption makes it seem as if both are averaged to 30 minutes. I also recommend the same use of colors as in Fig. 2, for consistency. Overall, however, it is a bit difficult to distinguish between the different experiments. Perhaps if both really are averaged to 30 minutes this will become clearer.

Yes, they are both 30 min average data. We have changed colors and data formats for a clearer view, see Figure 4 in the revised manuscript, also given below ('o' for the unused chamber and ‘Δ’ for the used chamber):

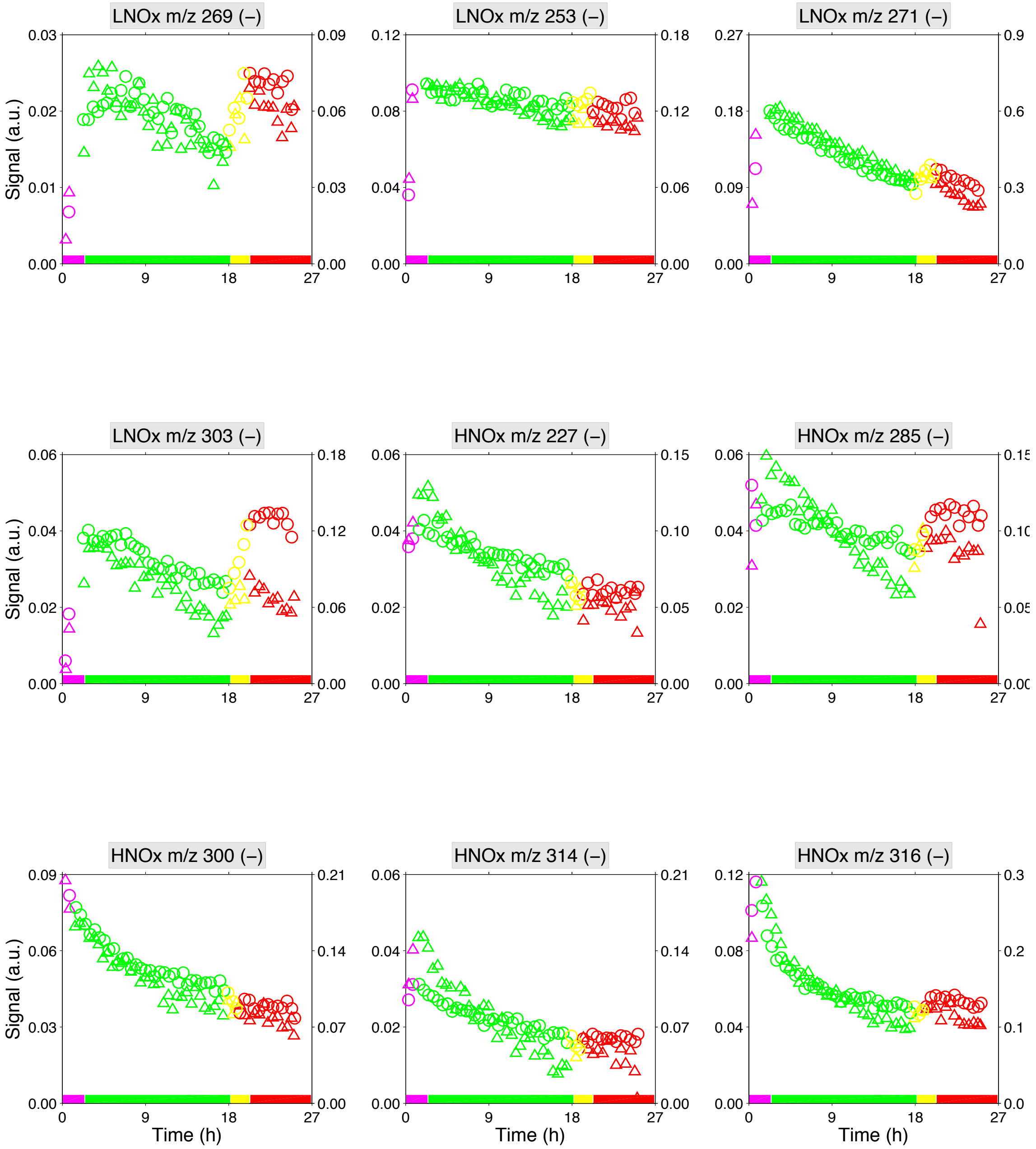


Fig. 4 and P26776: The authors note that “Their [Ziemann and Matsunaga’s] estimated Cw values are comparable with those derived from dodecane photooxidation products in the current study: : :”, and go on to mention two specific compounds. However, from Fig. 4 it is apparent that 5 compounds were considered for this system: the two explicitly mentioned but then 2 with much lower Cw values and one with a much higher Cw value. Thus, this statement seems overly general. Additionally, the authors might consider adding lines to Fig. 4 to indicate the range determined by Ziemann and Matsunaga.

It is a stretch to compare these two studies since there is no overlap between organic vapors detected. Thus, we have deleted this comparison in the revised manuscript. Instead, we have added comparison between a continuous decay over a relatively long time scale observed in this study and a rapid decay followed by the establishment of equilibrium over a relatively short time scale observed by Matsunaga and Ziemann (2010).

Eqn. 14: I'm sure the authors are simply being consistent with the literature, but it is a bit confusing when the subscript "H"s do not mean "Henry's Law". Why is "D" used? "Dissolution". The definitions are clearly stated, so this is not a problem per say, but simply a little confusing to the reader.

Yes, we kept the notation consistent with those in the material science literatures. It is a fair point that this notation be a bit confusing for the readers. We have revised the notation as follows:

$$C = C_{\mathrm{H}} + C_{\mathrm{L}} = k_{\mathrm{H}} p + \frac{C_{\mathrm{L}}' bp}{1 + bp} \tag{18}$$

"*…where* C *is the total vapor concentration in the glassy polymer,* C_H *is the concentration based on Henry's law dissolution,* C_L *is the concentration based on Langmuir sorption,* k_H *is the Henry's law constant,* p *is the partial pressure in the gas phase,* C_L' *is the hole saturation constant, and* b *is the hole affinity constant.*"

Eqn. 15: This equation does not follow from Eqn. 14. In Eqn. 14, the kD term is not multiplied by p, but in Eqn. 15 it is. There is a typo in one or the other. This has implications for Eqn. 16, if Eqn. 14 is correct.

Thanks for pointing it out. We corrected the typo:

$$C = (k_{\mathrm{H}} + C_{\mathrm{L}}' b)\, p \tag{19}$$

P26778: The authors conclude that the dependence of H on the saturation concentration implies a molecular weight dependence to solubility. It would be much more straightforward to simply graph H vs. MW to demonstrate this, as the figure (as currently presented) does not compellingly make the case, especially since there is only a loose relationship between molecular weight and vapor pressure since not all functional groups are created equally. Additionally, the authors focus their discussion here on molecular weight. But shouldn't the nature of the functional groups also play an important role on solubility? Can this be commented upon?

The vapor pressure depends ultimately on the size of the molecule, the functionalities attached, and their mutual interactions. The statement regarding "the dependence of solubility on molecular weight" is indeed too generalized. We revised this as "*This behavior suggests that organic vapor solubility in FEP films increases with decreasing volatility, i.e., increasing carbon number and functionalization.*"

Eqn. 17: As with Eqns. 12/13, the authors assume here that the maximum gas phase concentration (i.e. CIMS signal) is equal to Ctot, and thus Cw is simply the difference between Ctot and the instantaneous Cv. This does not take into account the possibility (or even likelihood) that vapors can be deposited to the walls during the photooxidation phase of the experiment, especially for the experiment with the longest photooxidation time (_7 hours). The authors should consider the implications that an underestimate in Ctot would have for their conclusions. As with the Cw/vapor pressure relationship, I can't help but think that some part of the derived alpha/vapor pressure relationship is potentially driven by differences in the influence of vapor wall deposition on the assumed total (vapor + wall) concentration.

We have addressed this issue earlier.

Also related to Eqn. 17, it is not entirely clear how the unit differences have been accounted for. Specifically, the Ctot and Cv terms are arbitrary, but Kw and Cw arenot. That said, the product Kw*Cw is dimensionless so it may not matter. But I suggest that the authors add some explicit statement here that indicates that they are using the CIMS signals with arbitrary units in their calculations.

Done.

"*Note that the product* $K_{w,i\ @T}C_w$ *is dimensionless, so that the normalized CIMS signal can be directly substituted into Eqs (16) and (17) as the actual gas-phase concentration of organic vapor i*".

The results from SIM.1 should be included in Fig. 2 in addition to the simulation results from SIM.3 (which is equivalent to SIM.2, apparently).

Done.

I do not necessarily agree with the conclusion on P26780 that the "outputs from SIM.3 [irreversible uptake] match the experimental data better than those from SIM.1 [reversible uptake] in general." Certainly there are a few compounds for which SIM.3 does a clearly better job: these tend to be the cases where the decay is visually linear with time and also the extent of loss (decrease from the max signal) is relatively small. But, there are also many cases where I think one could make an argument that the SIM.1 results do a better job. For example, the case shown in Fig. 2S, top left on the first page of Fig. 2S (m/z = 175). It is partly for this reason that I suggest the authors move the SIM.1 results to the main paper; this way the reader can more easily see the differences and decide for themselves which does a better overall job.

We have rewritten Section 6 'Accommodation coefficient on chamber walls' in the revised manuscript. Corresponding discussions are also shown below:

"*Simulations using both reversible (SIM.1) and irreversible (SIM.2) vapor wall deposition expressions match the experimental data. Outputs from SIM.1 tend to level off, whereas those from SIM.2 exhibit a continuous decreasing trend at the end of ~ 18 h of vapor decay. The extent of agreement between observations and simulations depends on the nature of vapor wall deposition: most organic vapors in the Caltech Teflon chambers exhibit a continuous decay. The agreement between SIM.1 and SIM.2 indicates that the estimated* C_w *values are sufficiently large so that the wall-induced vapor deposition in the Caltech chamber can be treated as an irreversible process* ($C_w \rightarrow \infty$) *within a relatively long timescale (<18 h)*".

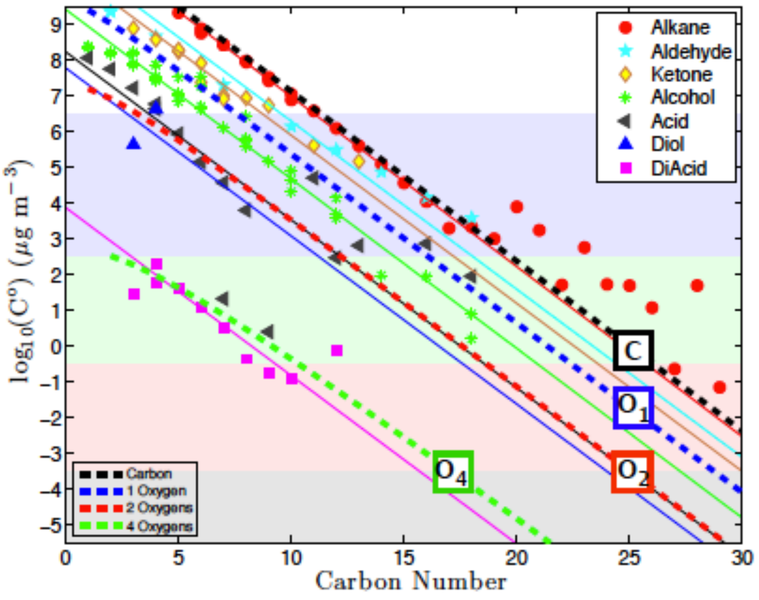
On P26781 the authors state: "The correlation of alphaw,i with the average carbon oxidation state (OSC), however, is not strong due to the fact that vapor pressures of small molecules, although highly oxidized, are not necessarily low owing to the short carbon backbone." This statement should be considered when the authors discuss the relationship between H and molecular weight on P26778 (and mentioned above).

We agree.

On P26781 the authors report an empirical relationship between alpha and C*. Given everything up to this point, I would have to assume that the C* values in Fig. 5 (as in Figs. 3 and 4), and used to deduce this relationship, were estimated from the EVAPORATION model. The authors then go on to report a relationship between C* and the number of carbon and oxygens in a molecule (Eqn. 21). It is not clear how well this expression reproduces the C*s from EVAPORATION. It seems to me that a critical aspect of allowing for combination of Eqn. 20 and 21 is that the C*'s are internally consistent. My concern here is that they are not. The authors need to clarify where the C* values in Fig. 5 (and Eqn. 20) come from (EVAPORATION or Eqn. 21). If they come from Eqn. 21, then this is inconsistent with what is shown in Fig. 3 and Fig. 4 (and presumably used the equations up to this point when estimating Kw values). If the C* values in Fig. 5 come from EVAPORATION, then the authors must demonstrate that Eqn. 21 and their derived vapor pressures from EVAPORATION are in good agreement. Alternatively, I suggest that the authors simply remove Eqn. 21 as it is unnecessary. The point being made in Fig. 6 can be made more generally just with words, without Eqn. 21.

The correlation of C^* with the carbon and oxygen numbers of a molecule (n_C/n_O), as shown in below, was first developed by Donahue et al. (2011). They have used vapor pressure data from NIST as well as the literature (Koponen et al., 2007; Cappa et al., 2007) to constrain this correlation, see the figure below. This volatility estimation approach, although quite simplified, proves to be very useful considering the fact that we have quite limited knowledge of the structure of organic aerosol constituents, whereas the measurement of the O:C and H:C ratios by AMS has become a routine procedure in many laboratories. In this way, one can reasonably constrain organic aerosol composition based on only two measurable or predictable properties, volatility and the extent of oxygenation.

$$\log_{10} C_{\mathrm{i}}^{*} = \left(n_{\mathrm{C}}^{0} - n_{\mathrm{C}}^{\mathrm{i}}\right) b_{\mathrm{C}} - n_{\mathrm{O}}^{\mathrm{i}} b_{\mathrm{O}} - n_{\mathrm{N}}^{\mathrm{i}} b_{\mathrm{N}} - 2 \frac{n_{\mathrm{C}}^{\mathrm{i}} n_{\mathrm{O}}^{\mathrm{i}}}{n_{\mathrm{C}}^{\mathrm{i}} + n_{\mathrm{O}}^{\mathrm{i}}} b_{\mathrm{CO}}$$



We suggest the the $\alpha_{w,i}$–C^*–n_C/n_O relationship is very important for the following two reasons: 1) While it is almost impossible to propose corresponding chemical structures for thousands of ions detected by mass spectrometry during an experiment, the proper guess of a molecular formula, coupled with the $\alpha_{w,i}$ – C^*– n_C/n_O relationship, would be able to constrain the wall-induced decay rate of each ion, and thus provide information to better understand its formation and removal dynamics, and 2) Some semi-explicit models, such as SOM by Cappa and Wilson (2012) or 2D-VBS by Donahue et al. (2011 and 2012), use the n_C/n_O pair to represent possible SOA-forming 'products' formed from the photooxidation of a parent hydrocarbon. It is useful to formulate an empirical relationship between the n_C/n_O pair and vapor wall loss rate so that the impact of vapor wall loss on the SOA yield can be estimated by such models.

Reviewer #2 has a valid point that the vapor pressure predictions from the C^* – n_C/n_O correlation might not be consistent with that estimated from the group contribution method. This discrepancy, however, is a result of the thermodynamic underpinning of the C^* – n_C/n_O correlation. For example, addition of one OH group leads to the decrease of vapor pressure of ~ 2.2 in the log scale, whereas addition of one C=O group leads only to the decrease of vapor pressure of ~ 1.0 in the log scale. However, the $C^* - n_C/n_O$ correlation uses a fixed value of 2.3 for the oxygen-oxygen interaction term, regardless of the structure of functional groups added. Further, volatility data were used to constrain the model performance in the development of both $C^* - n_C/n_O$ correlation and group contribution methods. Therefore, the empirical parameters obtained by optimizing the model output to the volatility measurements should represent the 'best' vapor pressure estimation under the current model framework. To verify this point, we have estimated the vapor pressures of 110 species, including C_5-C_{14} *n*-alkanes, C_5-C_{14} carbonyls, C_5-C_{14} di-carbonyls, C_5-C_{14} alcohols, C_5-C_{14} diols, C_5-C_{14} carboxylic acids, C_5-C_{14} di-carboxylic acids, C_5-C_{14} peroxides, C_5-C_{14} di-peroxides, C_5-C_{14} nitrates, and C_5-C_{14} di-nitrates, by taking the average from 'SIMPOL.1' and 'EVPORATION'. We then fit the $C^* - n_C/n_O$ correlation to the predicted vapor pressures. The best-fit parameters are given in the table below, together with those constrained by measured vapor pressure data (Donahue et al., 2011). We can see that the estimated parameters are reasonably close.

Parameters	This study	Donahue et al. (2011)
n_C^0	28.0483	25
b_C	0.4015	0.475
b_O	2.3335	2.3
b_{CO}	-0.4709	-0.3
b_N	3.6000	2.5

Minor: Page 26769: "an species" should be "a species"

Done.