Response to Reviews

Modeling secondary organic aerosol formation from volatile chemical products

Elyse A. Pennington[1,2], Karl M. Seltzer[1], Benjamin N. Murphy[3], Momei Qin[1,4], John H. Seinfeld[2], Havala O.T. Pye[3]
[1]Oak Ridge Institute for Science and Education Fellow in the Office of Research and Development, US Environmental Protection Agency, Research Triangle Park, NC 27711
[2]Department of Chemical Engineering, California Institute of Technology, Pasadena, CA 91125
[3]Office of Research and Development, US Environmental Protection Agency, Research Triangle Park, NC 27711
[4]Jiangsu Key Laboratory of Atmospheric Environment Monitoring and Pollution Control, Collaborative Innovation Center of Atmospheric Environment and Equipment Technology, School of Environmental Science and Engineering, Nanjing University of Information Science & Technology, Nanjing, China
Correspondence to: Havala O.T. Pye (Pye.Havala@epa.gov)

Anonymous Referee #1

General comment: This manuscript evaluates the role of VCPs in SOA formation by conducting CMAQ simulations with new VCP emissions inventory and chemistry. The results show that VCPs are one of the major sources of SOA in urban atmospheres, and they contribute half of anthropogenic SOA in modeled areas. The authors also address the uncurtains and limitations of CMAQ+VCP, illustrating the importance of a better understanding of VCPs. The manuscript is well written, and significant improvements have been made to SOA modeling. I have one major comment about the oxygenated IVOCs.
Thank you for all of the helpful comments. Each comment is addressed individually below.

Specific comment: The authors conclude that oxygenated IVOCs VCP precursors have a much smaller role in SOA formation from VCPs. However, this result is inevitable when you think about how the oxygenated IVOCs are treated in the CMAQ+VCP model. The authors use a single surrogate (SOAOXY) to represent the oxygenated IVOCs. It undergoes a one-step reaction with the hydroxyl radical to form a nonvolatile aerosol surrogate (AOIVOC). While the SOA yield for the oxygenated IVOCs ranges from 0.06 to 0.6, the lowest value was used for the SOA parameterization. I understand the challenges in modeling the oxygenated IVOCs in CMAQ, but it's not proper to have the statement that oxygenated IVOCs make fewer SOA from VCPs while the mechanisms of these compounds are not well-represented.
The SOA mass yield used to represent the SOAOXY → AOIVOC reaction (6.28%) was calculated by averaging the SOA mass yields of all individual VCP species assigned to SOAOXY, weighted by their emission fractions in Los Angeles County. While the SOA yields of the individual species range from 0% to ~60% (Figure S1), the species with lower SOA yields are emitted in higher quantities and have a larger impact on the net/averaged SOA yield. Fig. 3c indicates the nonoxygenated IVOC SOA is predicted to exceed the oxygenated IVOC SOA by about a factor of 10. So even if the highest individual oxygenated IVOC yield was applied to all oxygenated IVOCs, oxygenated IVOC SOA would not be expected to dominate. The overall SOA potential is a function of the individual SOA yields (uncertain given the lack of laboratory

and modelling studies), the composition of the SOAOXY (parameterized using LA County data), and also of the total emissions of SOAOXY (which will vary by location in the emissions inventories used). For example, in another location where SOAOXY was preferentially emitted compared to the nonoxygenated IVOCs, then it's importance would be elevated. The scope of our discussion about the impact of oxygenated IVOCs and siloxanes on SOA has been extended in Section 3.2:

> "While this work indicates oxygenated IVOCs form much less SOA than nonoxygenated IVOCs, more work is needed to determine if this result is robust across all emission sectors and in future conditions. Oxygenated IVOCs represent a class of emissions that has traditionally been discarded from regional models, but have become an important research focus with the rising importance of VCP emissions (Khare & Gentner, 2018). The contribution of oxygenated IVOCs and siloxanes to ambient conditions may be spatially variable and continue to evolve as product formulations shift towards exempt VOCs which tend to be oxygenated. Oxygenated IVOCs from other emissions sources, such as meat cooking or wood burning, could be abundant but were not considered here. Additionally, we do not know if SOA from these precursors has a health impact higher or lower than average $PM_{2.5}$."

Technical corrections:

P3, L70: "...SOA yields were reported under unrealistic atmospheric conditions", please add refs.
A reference to Charan et al. (2021) has been added, which discusses the issue of unrealistic atmospheric conditions in previous laboratory studies.

P3, L80: The abbreviation "CMAQ" has been introduced earlier in line 55.
This definition has been removed.

P4, L103: "...volatility(C*)", please provide a more accurate definition of C*.
"Volatility" has been replaced with "effective saturation concentration" here and in Section 2.2.

P4, L110: Cater, 2010 is cited here. Is it relevant?
This reference has been removed.

P5, L120~134: SAPRC07TIC_AE7I_VCP assignment rules are described quite well in the SI, but they are unclear to me in the main manuscript.
In response to this comment and a comment by Anonymous Referee #3, we removed the summarized list of assignment rules from the main text and now only reference the detailed assignment rules in the SI.

P7, L183: Please indicate the source of the SOA yield data in Figure S1.
References have been added to the caption of Figure S1.

P7, L185: The model species listed in Table 1 are unclear to me. Even though these species,

such as SILOX and SOAOXY, are included in the SOA chemistry, they undergo gas- phase reactions. Is that correct?
Yes, SILOX and SOAOXY undergo gas-phase reaction with OH to form lower volatility gas-phase (SVSILOX1, SVSILOX2) and particle-phase (ASILOX1J, ASILOX2J, AOIVOCJ) products. The phase state of these species were added to the main text and the footnotes of Table 1.

P7, L189: "...(SVSILOX2/ASILOX2J)", I only see ASILOX2 in the table, not ASILOX2J.
P7, L191: "...(SVSILOX1/ASILOX1J)", I only see ASILOX1 in the table, not ASILOX1J.
The labels in the first column of the table were extended to maintain consistent surrogate names.

P9, L235: In line 174, it said SOAOXY undergoes a one-step reaction with OH to form AOIVOC. However, SOAOXY is missing in Figure 1.
Surrogate names were added to Figure 1.

P11, L295: VCPs are predicted to be a larger source of IVOCs than mobile sources. Can it be quantified?
This sentence now includes a reference to Fig. S2 which depicts the gas-phase concentrations of IVOCs from the zero VCP case (including emissions of mobile and other non-VCP sources) and the CMAQv5.3.2+VCP case (including emissions from VCPs, mobile, and all other sources).

P14, L400: "...emissions and chemistry updates were approximately 5 times more effective than enhanced oxidant levels from VCPs in increasing SOA". I think this statement needs more discussion.
This discussion has been extended to include why ozone is used as a proxy for oxidation rates, as well as the impact on and relation to formaldehyde concentrations:

> "SOA can be facilitated by increases in oxidant abundance and chemical pathways from precursors to semivolatile or low-volatility products. Average noontime total SOA mass increased from 1.96 $\mu g\ m^{-3}$ in the zero VCP case to 3.62 $\mu g\ m^{-3}$ in the CMAQv5.3.2+VCP case (Fig. 3b), an increase of 84.7%. Ozone concentration can be used as an indicator of oxidant burden and oxidation rates due to its high responsiveness, while OH concentrations may be less responsive (Qin et al., 2021). The average noontime ozone concentration increased from 43.0 ppb in the zero VCP case to 49.2 ppb in the CMAQv5.3.2+VCP case (Fig. S3c), an increase of 14.4%. Assuming ozone can serve as a proxy for oxidation rates, the improved ozone concentration suggests that ~14.4% of increased model SOA concentrations are due to an increase in the oxidant burden and oxidation rates. The SOA mass increased by a larger percentage (84.7%), indicating emissions and chemistry updates combined were approximately 5 times [(84.7% - 14.4%) / 14.4%] more effective than enhanced oxidant levels alone in increasing SOA. This is consistent with the work of Qin et al. (2021), which found that the lack of key emitted precursors in models – rather than their associated radical chemistry – had the largest impact on $PM_{2.5}$ formation. Additionally, we note that the default CMAQ model (CMAQv5.3.2) with baseline chemistry and VCP emissions predicted about the same amount of SOA as the zero VCP case (Fig. S3a). In contrast, ozone increased in the default CMAQv5.3.2 model with VCPs (Fig. S3c). Since the oxidant burden increased noticeably in the CMAQv5.3.2 case but did not equate to a large

> increase in PM_1 SOA, results suggests the oxidant level alone does not have a large influence on enhancing SOA if the relevant precursor pathways are not also implemented.
>
> The response of formaldehyde can similarly be compared to the change in oxidant burden due to VCPs. At noontime, average formaldehyde increased from 2.41 ppb in the zero VCP case to 2.80 ppb in the CMAQv5.3.2+VCP case, an increase of 16.2%. As above, we attribute ~14.4% of the increase in pollutant concentration to the increase in oxidation rates. While formaldehyde does contribute to the oxidant burden via photolysis and radical initiation, the contribution of formaldehyde to the RO_x radical budget is likely small and on the order of 10% (e.g. Griffith et al., 2016; Kaiser et al., 2015; Luecken et al., 2018). Thus, the increase in formaldehyde concentrations between simulation cases is likely due primarily to the increase in oxidation rate. The increase in formaldehyde between simulation cases, therefore, cannot be largely attributed to the addition of S/IVOC emissions and their ability to form formaldehyde as a byproduct of oxidation. This is consistent with the work of Coggon et al. (2021), which showed that vehicle VOCs perturb formaldehyde to a larger degree than VCP VOCs do, suggesting that VCP emissions and fragmentation chemistry may not be directly responsible for formaldehyde, but rather modulate formaldehyde formation via changes in oxidant abundance."

P15, L419: "...Our results indicate", what results? Can you be more specific? In which figure or which table?
This sentence was rewritten to state the results (OA positively correlates with temperature, and the correlation is driven by SOA) and cite Fig. S7.

P15, L431: If SOA yield for the asphalt emissions can exceed 10% (the bias of SOA in CMQA+VCP is below 10%), will the SOA yield be over-predicted once this source is added to the model?
The SOA yield is defined as the mass of SOA formed divided by the mass of VOC precursor reacted, so the 10% yield is relative to the amount of emitted asphalt S/IVOC precursors. In contrast, the <10% bias in Fig. 5a relates to the amount of SOA formed relative to observed SOA. So, the percentages cannot be directly compared.

P17, L475~P18, L500: A few assumptions are made in these several paragraphs, but they are overturned immedicably by the authors. For example (line 477): "...which could result in a dilution effect matching the temperature dependence seen in Figure 5a. However, the predicted CO bias does not depend on temperature, which implies that modeled PBL height is not an important driver of the SOA bias temperature-dependence." I found this type of sentence is very confusing and suggest the authors rewrite these paragraphs.
Yes, that was confusing. Rather than presenting a possible explanation (error in predicted PBL height influencing error in predicted pollutant concentration) and then debunking that possibility, we condensed the PBL discussion into one sentence included in the paragraph about what the CO concentration bias can or cannot infer about the SOA bias. In other words, because the CO bias does not show a relation to temperature, errors in the modeled PBL height cannot describe the temperature-dependence of errors seen in predicted pollutant concentrations. We also added

more explanation to the topic sentence of the POA paragraph (beginning line 470) to better describe the purpose of that paragraph.

Anonymous Referee #2

This is an important study that models the role of VCPs in SOA formation. The study acknowledges current uncertainties and challenges to modeling the role of VCPs. The following points need additional discussions and clarifications:
Thank you for all of the helpful comments. Each comment is addressed individually below.

1. Line 145: What is the justification for assuming the VCP emissions profile peaks at noon and has no weekday-weekend differences?
The sinusoidal emissions profile is generally consistent with the more detailed diurnal profiles presented in Gkatzelis et al. (2021a), that were not available at the time of our modeling simulations. The diurnal variation of gas-phase IVOCs attributed to VCPs (Fig. S2) is consistent with that of the measured VCP dominated factor (Fig. 2 in Gkatzelis et al., 2021b), suggesting that the diurnal profiles used in this work are largely correct. Day-of-week variations in emission strength of VCPs has not been reported. Recent work using VCPy and CMAQ (Seltzer et al., in prep.) has utilized the diurnal profiles of Gkatzelis et al. (2021a).

2. Line 455: The slight increase in POA concentrations is with respect to what? This sentence needs rephrasing and clarification.
The slight increase in POA is seen between the zero VCP model predictions and the CMAQv5.3.2 model predictions. This has been clarified in the text.

3. Is POA considered semi-volatile and do different POA sources have different volatilities?
In our usage of CMAQ’s aerosol mechanism, inventoried POA from onroad and nonroad mobile sources are assigned to a volatility basis set (VBS) distribution as described in Lu et al. (2020). Fire, cooking and other anthropogenic combustion sources of POA are parameterized with source-specific reference volatility profiles as well. Some of the inventoried POA is in the condensed phase without any atmospheric chemical processing (considered POA) while some evaporates and undergoes gas phase oxidation resulting in SOA. When total OA loading increases (as seen between the zero VCP and CMAQv5.3.2+VCP cases), the amount of condensed POA increases according to partitioning theory. The source-dependence of POA volatility does not impact our results, since all POA emissions were constant in each of our model simulations (since VCPs do not emit POA in the VCPy model).

4. How does the modeled volatility distribution of SOA affect model-measurement bias with respect to temperature? Since the bias is shown to increase with temperature, is the modeled SOA too volatile? What is the role of particle-phase oligomer formation on volatility distribution of SOA from the dominant SOA sources?

A statement about the volatility of modeled SOA has been added to Section 3.3:

> "One possible explanation of the temperature-dependence of the SOA bias is that modeled SOA volatility is too high. But, oxygenated SOA is nonvolatile and nonoxygenated IVOC SOA is continually processed to lower volatility through gas-phase OH oxidation."

Particle-phase oligomer formation from the new VCP surrogates (siloxanes, oxygenated IVOCs, and nonoxygenated IVOCs) is not included in this model, but oligomerization reactions for the VCPs assigned to "traditional" model surrogates is included according to existing CMAQ chemistry (AOLGA and AOLGB in Fig. 1). Increased AOLGA/B mass due to VCPs is included in the mass of traditional model surrogates (Fig. 3c). While the new VCP surrogates do not consider oligomerization explicitly, the oxygenated IVOC SOA is nonvolatile which should lead to overestimates at high temperature if volatility were an issue. In addition, the nonoxygenated IVOC SOA is continually chemically processed to lower and lower volatility which could mimic the volatility of oligomerized SOA. There have been no laboratory or modelling studies performed to investigate the role of oligomerization reactions from VCPs or other S/IVOCs, and this has been added to Section 3.2 as another remaining source of uncertainty in these models.

5. Why is modeled formaldehyde higher in CMAQ+VCP case compared to zero VCP case? Is this related to increase in radicals and ozone in the CMAQ+VCP case that increase formaldehyde production as temperature increases?
We calculated the impact of oxidant burden on increased formaldehyde concentrations (see Section 3.2 and the response to Anonymous Referee #1's comment "P14, L400" above) and found that the increase in formaldehyde concentrations between simulation cases is likely due primarily to the increase in oxidation rate, which you correctly identified as increasing with increasing temperature. This means that the statement in Section 3.2, "The increase in formaldehyde was predominantly due to the increased magnitude of VCP emissions", is incorrect. It has been removed and the formaldehyde increase is discussed further in Section 3.3. However, this source apportionment of formaldehyde error compared between cases does not explain why the HCHO bias (in all simulation cases) decreases with temperature. This discussion is continued in response to comment #6 below.

6. Line 495: It is not clear to me if we can make a general statement that formaldehyde is an important indicator of SOA formation. First, SOA products have a range of volatitlies, and ultimately SOA could be lower volatility than currently assumed (see comment 4). In contrast formaldehyde is volatile. Secondly, the chemistry for SOA products is much more complex than formalehyde. One could likely say VCP-SOA precursor emissions could correlate with formaldehyde as a function of temperature.
This discussion has been revised at the end of Section 3.3:

> "In contrast to POA and CO, the formaldehyde bias demonstrated the same trend with temperature as SOA (Fig. 5c). This suggests that formaldehyde is affected by emissions, chemistry, and dilution changes similarly to SOA. This is supported by the stronger correlation seen between SOA and formaldehyde compared to the correlation between SOA and POA or CO (Fig. S8). Therefore, formaldehyde may provide more information about the errors in modeling VOC chemistry and possibly SOA formation. It is possible that remaining formaldehyde bias is due to missing formaldehyde emissions. The VCP inventory includes

near-zero emissions of formaldehyde, but formaldehyde is emitted from wooden furniture and emission rates increase with temperature (Wang et al., 2021). This may account for some of the temperature-dependence of formaldehyde bias, but likely not the entirety since the VCP emissions inventory has been evaluated with select ambient VOC measurements with low error (Seltzer et al., 2021). One possible explanation of the temperature-dependence of both the SOA and formaldehyde biases is missing sources of emissions and resulting chemistry. Previous work has shown that formaldehyde formation is particularly sensitive to the emissions/chemistry of alkenes (e.g. isoprene) and, to a lesser extent, alkanes and aromatics (Luecken et al., 2018), so these precursors likely indicate missing emissions as a source of error in our model. While the radical chemistry of these hydrocarbon precursors are included in the model, additional missing chemistry may be causing some of the error. Chemical processes that have not been included in the mechanism include autooxidation (Crounse et al., 2013) – which forms low-volatility SOA – and formaldehyde potentially formed from the fragmentation of S/IVOC precursors to SOA. The inclusion of these missing emissions and/or chemistry would further impact oxidant levels, which we have shown to be an important source of modeled SOA and formaldehyde. As stated above, the behavior of POA and CO bias suggest that errors in combustion emissions and PBL height cannot fully describe the temperature-dependence of SOA bias, and POA and CO are better indicators of mobile and industrial sources. Formaldehyde may instead serve as a better indicator of SOA production in urban areas where VCPs are important atmospheric constituents. While many factors may contribute to the temperature-dependence of SOA and formaldehyde bias, future work must investigate the importance of these factors and tracking the response of formaldehyde to these changes alongside SOA could provide insight. ”

7. Given the motivation mentioned a role of oxygenated VOCs, it was surprising that oxygenated VOCs have much smaller role in SOA formation from VCPs. Same is the case for siloxanes. Can one neglect the role of siloxanes and oxygenated VOCs in SOA formaton from VCPs? This needs more discussion.
Please see the response to Anonymous Referee #1’s second comment (specific comment) above regarding oxygenated IVOCs, and the discussion added to Section 3.2.

Anonymous Referee #3

This manuscript describes a modeling effort where VCP emissions are included into CMAQ. Overall, inclusion of these emissions improves predictions of SOA, HCHO, and O3 concentrations, though SOA remains under predicted.
Thank you for all of the helpful comments. Each comment is addressed individually below.

Overall the manuscript is well written and is an important contribution. My main concern is that, as written, the manuscript seems to rely on readers having a good working knowledge of the VCPy inventory. I think adding more detail on the inventory in a few key places will help readers to better understand the findings of this study (without having to refer back to Seltzer et al several times). Tow examples of this are:

1. **Presumably VCPy is both spatially and temporally resolved. The temporal resolution seems to be especially important, since there seems to be some evidence that personal care product VCPs have stronger emissions in the morning than later in the day. It would be worthwhile to spend a few sentences on some of the important temporal profiles of VCPs.**
   Please see the response to Anonymous Referee's comment #1 above.

2. **I think the discussion of temperature-dependent biases in Fig 5 would also benefit from more detail on the emissions. It seems like the added VCP emissions include some temperature-dependent evaporative emissions (hence improvements in bias relative to the no-VCP case at higher temperature), but that some sources may be missing (since the bias at high temperature is still large). Right now there is a text description of some of these trends; it would be helpful to have a figure showing how some of the VCP emissions perhaps vary with temperature and/or time of day.**
   The temperature-dependence of VCPy emissions is for now limited to our understanding of time-of-day profiles, as explained by the relation to Gkatzelis et al. (2021a). In the VCPy model, a temperature of 298 K is assumed to calculate the volatility of VCP species and hence annual emission rates. This temperature is accurate for indoor emissions, but the temperature-sensitivity of outdoor emissions could be a focus of future work.

Other comments:

I'm not sure what is meant by "these alkane surrogates" in line 129. I thought the point was to reallocate IVOCs into classes that form SOA.
In response to this comment and a comment by Anonymous Referee #1, we removed the summarized list of assignment rules from the main text and now only reference the detailed assignment rules in the SI.

Figure 1 - it would be good to explicitly state what parts of this map are new to this work. I think it's everything in orange font.
The caption has been extended to state that the thick red boxes represent the part of the mechanism that is specific to this work.

Fig 4b and 4c could benefit from including the 1:1 line.
This has been included.

Non-oxygenated IVOCs contribute the most to the additional SOA made in the "with VCP" case (e.g., Fig 4c). What are the major sources of these emissions?
The most abundantly emitted nonoxygenated IVOCs were C12-C16 straight-chain alkanes, C12-C16 cycloalkanes, and fragrances. The dominant sources of these compounds were printing inks, general cleaners, daily use products, and allied painting products (Seltzer et al., in prep.).

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