

Geosci. Model Dev. Discuss., referee comment RC1
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Comment on gmd-2022-90

Anonymous Referee #1

Referee comment on "A lumped species approach for the simulation of secondary organic aerosol production from intermediate-volatility organic compounds (IVOCs): application to road transport in PMCAMx-iv (v1.0)" by Stella E. I. Manavi and Spyros N. Pandis, Geosci. Model Dev. Discuss., <https://doi.org/10.5194/gmd-2022-90-RC1>, 2022

General Comments

This study presents a new model to represent the IVOC emissions and SOA formation from on-road gasoline and diesel vehicles in Europe. A SAPRC-based model using 7 new surrogate species was developed based on experimental emissions and smog chamber data. This study shows that IVOC emissions have previously been underestimated by a factor of 8, and the new model surrogates have higher SOA yields than existing VOC model surrogates. The paper does a good job of describing how the new model was developed, but I have a few general questions about the Introduction and Conclusion, and recommendations for how to reorganize some of the information.

Specific Comments

In this paper you focus specifically on IVOCs. Can you please add a statement in the Introduction stating why you do not investigate SVOCs, LVOCs, or ELVOCs? In Section 2.2 (line 104), you state that the existing PMCAMx VBS model includes volatility bins reaching to $0.01 \mu\text{g m}^{-3}$, so it would be good to specifically (briefly) address those compounds as well. I believe lower-volatility species simply were not included in the Zhao work that your model is parameterized on?

Line 26-28: Emitted/primary IVOCs also include oxygenated compounds, although these tend to not be emitted from vehicles.

Line 44: "due to their size and low volatility"

Lines 63-79: Please give more description why the models described here, which use the same experimental dataset, are insufficient. For example, the model from Lu et al., 2020 already separates the IVOC emissions by C^* , k_{OH} , MW, SOA yield, and structure (alkane vs. aromatic). Your model further separates IVOCs into more specific structural categories, which is a difference worth explicitly mentioning in this paragraph and the Conclusion.

Table 1 is very detailed and may be more appropriate for the SI. Table 1 could instead just give the properties of the 7 new surrogates used in the model (C^* , k_{OH} , MW, SOA yields/ a_i).

Reference Table 1 (or Table S1, if you move it to the SI) in the second paragraph of Section 2.3 to introduce your descriptions beginning in line 122.

Line 175-177: This is somewhat vague. State explicitly here what the "more volatile products of the reactions" are or state what the "larger lumped VOCs that are already present in the SAPRC mechanism" are. This may warrant an extra table in the SI matching up existing surrogate products with the new surrogate products, or reference the code provided in the Data Availability section.

Lines 182 and 194: Are the OCG_i species the same as the 5 products that you reference in lines 173-174?

Lines 189 and 198: The reactions of ALK7-ALK9 and PAH1-PAH2 should be given somewhere (an in-text or SI table, or referenced to the code provided in the Data Availability section).

I recommend reorganizing Sections 2.4.1-2.4.3 and 2.5. Presenting the information more chronologically could be helpful. Reference Section 2.5 in the two sentences in lines 206-209.

Line 300 and Figure 1: Are the spatial and temporal distribution of the IVOC emissions determined by the GEMS inventory given in line 292? The spatial and temporal distribution warrant more description since you present the maps in Figure 1.

Consider adding figures to the SI for all new surrogates which match the information given in Figures 2 and 3.

Line 353: "Estimated based on experimental data and the fitting algorithm"

Lines 355-356: These yields do not match the values given in Table S3. Are these values from the fitted line?

Lines 408-409: Add reference to the last statement.

Lines 413-414: A benefit of your model is that it matches the same surrogate+reaction scheme of the existing SAPRC model, so it could be easily integrated into existing SAPRC models rather than integrating an entirely new VBS or other model. I think this benefit should be more explicitly stated in the Conclusion.

Can you provide a quantitative estimate of how much this model could increase predicted SOA mass in Europe? In lines 427-230 you state that a subsequent study will apply the model, but using the results in this paper you can predict a bulk percent increase of SOA mass over Europe.

Technical Corrections

All: Some of the in-text citations use et al. and others use et al

Lines 89-90: Replace "on" with "to" to avoid the repetition of "on on-road": "In this work, the proposed IVOC scheme is applied to on-road transportation and more specifically to IVOCs emitted by diesel and gasoline vehicles following the studies of Zhao et al. (2015; 2016)."

Line 93: Name the version of SAPRC, e.g. SAPRC07 or SAPRC99.

Line 166: "below"

Line 201: Be consistent with the tense used. "includes" should be "included".

Line 296: Define the EUCAARI acronym and give a reference.

Figure 4: Rename x-axis label "Old" to "Old VBS" for clarity and consistency with the text.

Figure 7: a_i (subscript)

Figure 10: Add legends.

Lines 415-416: "...compared to the IVOC emissions previously used, which assumed that they were equal to..."

Line 417: "15%"

Line 418: You use MS/GC without defining the acronym, but in line 32 you use gas-chromatograms.

In the Zenodo link, correct "were" to "where" in the description and correct the title.