

Interactive comment on “Modelling organic aerosol concentrations and properties during ChArME_x summer campaigns of 2012 and 2013 in the western Mediterranean region” by Mounir Chrit et al.

Anonymous Referee #2

In this work, Chrit et al. used a mechanistic model to describe the biogenic secondary organic aerosol formation and properties at a measurement supersite in Corsica during two summer campaigns. They found that the consideration of ELVOCs and organic nitrates greatly improved the simulated OA concentrations and oxidation state. This study is of definite interest to the ACP audience by contributing to the organic aerosol modeling field and the scientific methodology used sounds valid. Overall, the manuscript is very well written and the presentation is clear. Therefore, I recommend this study for publication. Below are a few minor comments to be considered prior to publication.

Specific comments:

1. Page 2 line 12: Delete “secondary” before “semi-volatile” and add intermediate volatile organic compounds (IVOCs) as another potential source of SOA.

The sentences “OA are classified either as primary (POA) or as secondary aerosols (SOA). POA are directly emitted in the atmosphere, whereas SOA are produced through chemical oxidation of volatile organic compounds (VOCs) and secondary semi-volatile organic compounds (SVOCs). SOA are often semi volatile, i.e. they partition between the gas and particle phases.” are replaced by “OA are usually classified either as primary (POA) or as secondary aerosols (SOA). POA are directly emitted in the atmosphere, often as intermediate/semi-volatile organic compounds (I/S-VOCs), which partition between the gas and the particle phases (Robinson et al., 2007). The gas-phase I/S-VOC are missing from emission inventories (Couvidat et al. 2012, Kim et al. 2016). SOA are produced through chemical oxidation of volatile organic compounds (VOCs) and I/S-VOCs, and condensation of I/S-VOCs.

2. Page 4 line 33: Can you please briefly describe (e.g., using a table) the surrogate species that you are using to represent the SOA formation from these five classes of precursors?

A table of the five classes of precursors is added in the revised paper:

| Precursors | Surrogate species |
|----------------|---|
| I/S-VOC | 3 volatility bins : $\log(c^*) = -0.04, 1.93, 3.5$ with c^* the saturation concentration. |
| Aromatics | Toluene, xylene |
| Isoprene | Isoprene |
| Monoterpenes | α -pinene, β -pinene, limonene |
| Sesquiterpenes | Humulene |

3. Page 5 line 23: It would be interesting to consider this lower yield in your sensitivity analysis.

It is possible to infer a lower and upper bound from the papers of Ehn et al. (2014) et Jokinen et al. (2015), as shown in the Table below.

| VOCs | Ehn et al. (2014) | Jokinen et al. (2015) |
|------------------|-------------------|-----------------------|
| α -pinene | 7% \pm 3.5% | 3.4% \pm 1.7% |
| Limonene | 17% \pm 8.5% | 5.3% \pm 2.6% |

Details on the ELVOC yield and the choice of the bounds are added in section 2.2. The sentence “ELVOC is assumed to be formed with an average molar yield of 11% following Ehn et al. (2014), although Jokinen et al. (2015) reported lower yields (about 5%).” is replaced by “The ELVOC yield is assumed to be 11%, i.e. close to the average of the yields of α -pinene and limonene according to Ehn et al. (2014). Jokinen et al. (2015) suggested lower yields (Table 2). In this paper, sensitivity simulations with a lower bound of 3% and an upper bound of 18% are also conducted”.

The following sentences are added in section 4. “Two sensitivity simulations are performed using a lower bound yield (3%) and an upper bound yield (18%). In Appendix D, similarly to what is presented in this section for the reference simulation, the sensitivity simulations are compared to each other and to the measurements in terms of the mass of OM₁, the organic aerosol composition, the OM:OC and O:C ratios.

4. Page 6 Table 1: Are the reported saturation vapor pressures of organic nitrates and MBTCA also at 298 K? If so, please add the “298 K” at the column head.

The “298 K” is added for the reported saturation vapor pressure of MBTCA in table 1 of the revised paper.

5. Page 8 line 20: Does this ratio also include the IVOCs? If so, please rewrite as (SVOC+IVOC)/POA

For clarity, the sentences “POA are assumed to be the particle phase of semi-volatile anthropogenic organic emissions (SVOC). Total SVOC emissions are estimated as detailed in Couvidat et al. (2012), by multiplying POA by a fixed value, and by assigning them to species of different volatilities. In this study, the ratio SVOC/POA is set to 2.5 (Kim et al., 2016; Zhu et al., 2016). Setting the ratio SVOC/POA to 1 has little impact on the organic concentrations” are replaced by “POA are assumed to be the particle phase of I/S-VOC. Total I/S-VOC emissions (gas and particle phases) are estimated as detailed in Couvidat et al. (2012), by multiplying POA by a fixed value, and by assigning them to species of different volatilities. In this study, the ratio I/S-VOC/POA is set to 2.5 (Kim et al., 2016; Zhu et al., 2016). Setting the ratio I/S-VOC/POA to 1 has little impact on the organic concentrations, as shown in Figure 5.”

6. Figures 3 and 6: Please consider improving the quality of the figures (e.g., font size, shape of pies, etc.).

The quality of the figures is improved in the revised paper.

References:

Couvidat, F., Debry, É., Sartelet, K., and Seigneur, C.: A hydrophilic/hydrophobic organic (H₂O) model: Model development, evaluation and sensitivity analysis, J. Geophys. Res., 117, D10 304, doi:10.1029/2011JD017214, 2012

Ehn, M., Thornton, J., Kleist, E., Sipilä, M., Junninen, H., Pullinen, I., Springer, M., Rubach, F., Tillmann, R., Lee, B., Lopez-Hilfiker, F., Andres, S., Acir, I., Rissanen, M., Jokinen, T., Schobesberger, S., Kangasluoma, J., Kontkanen, J., Nieminen, T., Kurtén, T., Nielsen, 10 L. B., Jørgensen, S., Kjaergaard, H. G., Canagaratna, M., Dal Maso, M., Berndt, T., Petäjä, T., Wahner, A., Kerminen, V., Kulmala, M., Worsnop, D. R., Wildt, J., and Mentel, T. F.: A large source of low-volatility secondary organic aerosol, *Nature*, 506, 476–479, doi:10.1038/nature13032, 2014.

Jokinen, T., Berndt, T., Makkonen, R., Kerminen, V., Junninen, H., Paasonen, P., Stratmann, F., Herrmann, H., Guenther, A. B., Worsnop, D. R., Kulmala, M., Ehn, M., and Sipilä, M.: Production of extremely low volatile organic compounds from biogenic emissions: Measured yields and atmospheric implications, *Proc. Nat. Acad. Sci.*, 112, 7123–7128, doi:10.1073/pnas.1423977112, 2015.