

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

## **Anonymous Referee #1**

Received and published: 13 July 2017

Review of Chrit et al. This paper models the organic aerosol concentration and properties during the ChArMEx summer campaigns of 2012 and 2013 using a surrogate approach for SOA formation. Although I agree with the importance of this topic and its novelty, the modeling approaches need to be clearly explained. Also, the caveats of these approaches need to be better acknowledged. Below are my specific comments that should be addressed before the paper is accepted for publication. 1. The abstract mentions that surrogate species for monoterpenes are  $\alpha$ -pinene and limonene. But on page 5, the authors mention three precursors:  $\alpha$ -pinene,  $\beta$ -pinene and limonene. This

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needs to be clarified. Also, why were these 2 particular species chosen as surrogates for monoterpenes?

2. Page 3: Why was IEPOX not observed during ChArMex campaign? Did the instruments measure gas-phase IEPOX or particle phase iepox components? Was the aerosol acidic or neutral?

3. The authors mention the importance of organosulfates in this study. But IEPOX chemistry also makes organosulfates. If these are not coming from isoprene or IEPOX chemistry, what are alternate mechanisms for organosulfates from monoterpenes or sesquiterpenes? Adding some discussions and references regarding this point would be helpful.

4. Page 4 and 11: In this study, did the authors use VBS for SVOC/IVOC species? Did they account for fragmentation and non-volatile SOA? Details regarding this approach need to be added. Also, note that the Cholakian et al. (2017) paper is not available online. Was the treatment of fragmentation and non-volatile SOA similar or different than other papers, for example: [M. Shrivastava et al., 2015; M. Shrivastava et al., 2013].

5. Page 11: What are IVOC/POA emissions assumed in this study? Was oxygen added during aging? How was fragmentation treated? Do their aging mechanisms include NO<sub>x</sub>-dependence?

6. Page 6: Organic nitrates: How uncertain are the reaction mechanisms and reaction rates for organic nitrate formation? The authors mention organic nitrates were not measured during ChArMex. But, it would be useful to point out what are the most important routes for organic nitrate chemistry mechanism: e.g. relative importance of nighttime TERPNRO<sub>2</sub> versus daytime TERPRO<sub>2</sub> reaction with NO. Also if this mechanism has been validated against other field campaigns in other papers, those references need to be added.

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7. Figure 4: What is contribution of SVOC/IVOC to evolution of OM:OC ratio and O:C ratio?

8. Page 14: Discussions on water soluble organics should acknowledge pathways other than organic nitrate to formation of water soluble species. For example, biomass burning sources (if significant), other SOA chemistry e.g. formation of organic salts, aqueous phase and cloud processing etc. See the recent review article on SOA [Shrivastava et al., 2017].

9. Page 20: Hydrolysis is mostly interpreted as a loss mechanism. But Pye et al. 2015 referred to it as pseudo-hydrolysis of organic nitrates that makes them non-volatile. Please clarify if this is what is being referred to.

10. Hydrophilic properties could change not just due to the hydrophobicity of organic nitrates. It could point to other mechanisms and SOA pathways not considered in the model e.g. aqueous and cloud chemistry, other SOA pathways like organic salts, organic-inorganic interactions etc. It is important to make sure the model is getting the right answers for the right reasons.

References: Shrivastava, M., et al. (2017), Recent advances in understanding secondary organic aerosol: Implications for global climate forcing, *Rev. Geophys.*, 55(2), 509-559, doi:10.1002/2016RG000540.

Shrivastava, M., et al. (2015), Global transformation and fate of SOA: Implications of low-volatility SOA and gas-phase fragmentation reactions, *J. Geophys. Res.-Atmos.*, 120(9), 4169-4195, doi:10.1002/2014jd022563.

Shrivastava, M., A. Zelenyuk, D. Imre, R. Easter, J. Beranek, R. A. Zaveri, and J. Fast (2013), Implications of low volatility SOA and gas-phase fragmentation reactions on SOA loadings and their spatial and temporal evolution in the atmosphere, *J. Geophys. Res.-Atmos.*, 118(8), 3328-3342, doi:10.1002/jgrd.50160.

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