

Interactive comment on “Investigating the links between ozone and organic aerosol chemistry in a biomass burning plume from a prescribed fire in California chaparral” by M. J. Alvarado et al.

Anonymous Referee #2

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The paper presents an updated version of the atmospheric chemistry box model – Aerosol Simulation Program (ASP) and its application to a young biomass burning (BB) plume. Simulation of NO_x, PAN, O₃, organic aerosol (OA) and other chemical species, and their comparison with the observations are presented. So far atmospheric chemistry models have been struggling to accurately reproduce the ambient OA concentrations. One of the objectives of this modeling study is to improve our understanding of the secondary OA (SOA) formation and evolution within BB plumes. The state of the art volatility basis set approach has been implemented in the ASP model to simulate SOA concentrations. Different variations of the SOA parameterization are tested in this

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study. Given the scientific importance of understanding the BB impact on air quality and climate, I think this modeling study deserves a publication. However, the authors need to do some reworking before the paper can be suitable for ACP.

My major comment on the study is the treatment of the SVOC chemistry in the ASP model. To my knowledge, majority of the atmospheric models treat the SOA chemistry independently from the gas chemistry. Here, the authors introduce some chemical reactions for the SVOCs (p. 32438). These reactions are intended to improve the gas phase chemistry simulations along with the SOA simulations. First of all, the authors need to make clear, what laboratory studies are these reactions (e.g. R4) based on? The SVOCs can comprise myriad of different type of molecules, and without knowing their chemical structure how one can treat their reaction products more “explicitly”? For instance, what VOCs are made by the reaction R4?

The chemical mechanism for the SVOCs and the parameters optimized here are for the Williams fire. Will the same model work for simulations of gaseous and aerosol species in another BB plume?

SVOCs are briefly defined in P. 32429. I think it needs to be made clear whether intermediate VOCs (IVOCs), which are important SOA precursors are included here as a part of SVOCs. Additional literature needs to be discussed regarding this point. If IVOCs were part of SVOCs in the model, then how accurate would be to assume the same chemical reactions (e.g. fragmentation rate) for the chemical compounds with very different volatilities and oxidation degrees?

You used the estimates by Grieshop et al. for initial SVOC concentrations (Table 4). Then you show that the ASP model overestimates the SOA concentrations, especially using the Grieshop et al. parameterization. In order the model to match the observations of OA strong fragmentation pathways for SVOC oxidations are assumed here. The SVOC species oxidize and contribute to the SOA increase downwind. Therefore, a question arises; maybe the initial SVOC concentrations for the BB plume are overes-

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timated in the model? I agree that introducing fragmentation in the SOA model makes sense, but as the authors noted the fragmentation used here may be unrealistically too high.

You used carbon monoxide (CO) to determine the best-fit model parameters for the dilution. This implies that CO was assumed to be completely a passive tracer. What about the chemical production and loss of CO within the fire plume? How much uncertainty does this approach introduce in determining the dilution rates, consequently in simulating other gaseous or aerosol species?

Figure 5: To calculate the enhancement ratios for O₃ CO, while for PAN CO₂ species are used. Why not to use the same species (e.g. CO) across the paper for consistency?

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