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Interactive comment on "Multi-generational oxidation model to simulate secondary organic aerosol in a 3-D air quality model" *by* S. H. Jathar et al.

Anonymous Referee #2

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The paper describes the implementation of a new parameterization (SOM) describing the formation of secondary organic aerosols (SOA) in a 3D air quality model (UCD/CIT). The aim is to describe the gas phase multi-generational oxidation of organic species leading to SOA formation based on an empirical approach. In this study, the SOM model is connected with the SAPRC chemical mechanism and simulations are performed for 2 summer week periods in the south coast air basin of California and the eastern United States. This paper presents a new tool and I think it is appropriate for publication in GMD. However, I have few major comments that the authors should consider for the production of a revised paper.

My major objection concerns SOA formation in SOM as a function of NOx levels. Two

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SOM grids are available, one for low NOx conditions (high SOA yields) and another for high NOx conditions (low SOA yields). These two grids are used successively over the full domain. Using two sets of results based on these two distinct grids is not satisfactory in the perspective of model applications. The paper states that the "current configuration does not allow for continuous variation in the dependence of SOA on NOx" (p1870, l27). This is clearly a major weakness of this model configuration. This paper being devoted to the implementation of SOM in 3D models, the authors should explain how SOM can ultimately be used to simulate the range of NOx conditions (i.e. from high to low NOx) encountered in a given domain. This point is a critical issue that should be examined in this paper devoted to SOM implementation, i.e. how could the model configuration be improved, can a "unified" parameterization (from low to high NOx conditions) be designed based on a these two grids . . .

The authors claim that the SOM version tested in this study does not account for oligomerization or heterogeneous reactions (e.g. p1869, l22-27). This statement is misleading. Indeed, the SOM approach is empirical, based on chamber observations in which these processes very likely occur. Even though no transformation in the condensed phase is explicitly represented in the design of SOM, fitting SOM to match chamber observations somehow implicitly account for these processes. The links between SOM design, chamber observation fits and 3D applications deserve additional discussion in the paper.

Minor comment: The sentence p1878, l21 is ambiguous. The high NOx and low NOx grids were alternatively used over the full domain, without considering the simulated NOx field (see also comment above). How can the authors state that the "product distribution is different under different NOx levels"? A "unified NOx parameterization" should be used to answer this question.