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Atmospheric Chemistry and Physics Discussions

Interactive comment on "Explicit modeling of organic chemistry and secondary organic aerosol partitioning for Mexico City and its outflow plume" *by* J. Lee-Taylor et al.

Anonymous Referee #2

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The manuscript describes the simulation of organic aerosol in Mexico City using a near-explicit photochemical chemical scheme in a 0-D model framework. It presents a fairly comprehensive discussion of the relative contributions of precursors to the magnitude and elemental compositions of modelled organic aerosol. The various sections of the manuscript are well laid out and easy to read and follow. In my view the material presented here gives additional useful insight in the modelling of organic aerosol and I recommend publication in ACP after the following clarifications and corrections are made.

General Comments

1. Page 17017, line 15 and discussed on page 17037 lines 23-27: The authors are using the vapour pressure equation of Myrdal and Yalkowsky with the Tb estimation method of Joback and Reid. This Tb estimation method has been repeatedly shown to give too high boiling points (for Tb values above about 550K) leading to a substantial underestimate in vapour pressure and consequently enhanced SOA mass. Why this choice when the authors know it overestimates SOA?

2. Page 17017 lines 15/16:- The Myrdal and Yalkowsky equation is not a group contribution method. Suggest this sentence is reworded to read ....using the method of Myrdal and yalkowsky (1997) with boiling points estimated using the group contribution method of Joback and Reid (1987) with the...

3. Page 17018, lines 18-20: why were nonadecane and eicosane reactions allowed to react to fifth generations (and 3rd generation for larger NMHCs). Is this for scientific or practical reasons?

4. Page 17020, line 7: "coeffiecients" should be "coefficients".

5. Page 17020, lines 8-9: The decision to neglect wet and dry deposition is odd. Were there any sensitivity studies that were done to validate this?

6. Page 17021 line 7 and Table 2 on page 17056: Assuming zero background concentrations of VOCs such as ethane, propane etc does not seem right as it has the potential to perturb the simulated radical budget. Any justification for this and/or an explanation in your discussion how such an assumption would affect the conclusions.

7. Page 17024 line 6: By how much is 2-pentene underrepresented in the emissions parameterisation and what is the impact in the simulated organic aerosol?

8. Page 17032, lines 13:16: Given the significant contribution of biogenic precursors to SOA, the omission of biogenic species is regrettable. Biogenics may be lower in concentrations that anthropogenics in Mexico City but they still have higher potential to impact SOA and thus, changing the magnitude and the elemental composition of

simulated SOA. Perhaps the title could be changed to reflect that this is anthropogenic organic chemistry study?

9. Page 17038, line 3 should be "agreement"

10. Figure 1 caption is inadequate for this figure and needs to be improved with some explanation provided for all the lines

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Interactive comment on Atmos. Chem. Phys. Discuss., 11, 17013, 2011.