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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 #1

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This manuscript describes the application of a detailed (nearly explicit) photochemical box model to the simulation of Mexico City organic aerosol and investigates the simulated concentrations, elemental composition and relative contributions of precursors over Mexico City and downwind. The paper is quite clear and easy to follow, particularly in light of the complex model set-up and analysis. It also included a comprehensive discussion of the robust conclusions and uncertainties which was very balanced and thoughtful. I have some minor points below, mainly to add some clarifications. I recommend that this manuscript be published in ACP once these comments have been addressed.

Minor comments

1. Abstract, line 14 and page 17038, line 20: specify that the larger n-alkanes are estimated SVOC precursors

2. Page 17015, line 17: Technically, field observations do not measure SOA, the AMS analysis identifies OOA and HOA. Similarly, while SOA mass increases were postulated by de Gouw et al., this was not strictly measured. I suggest you re-phrase.

3. Page 17016, lines 9-10: "improved agreement" is a little vague – could you specifically state that these treatments reduced the model bias?

4. Section 1: The discussion of Section 4 answered many questions that came up as I read this manuscript. It would perhaps be worth noting explicitly at the end of Section 1 that you will discuss uncertainties and limitations in the model treatment in Section 4, so that the reader knows that they can expect this.

5. Page 17020, line 10: It would be nice to have the justification for neglect of dry deposition spelled out a bit. In particular, it seems that some gas phase organics would have significant dry deposition rates. Could you provide some values to compare to kent and kvent? It might be useful to indicate that this will be discussed further in Section 4.4 or move that discussion of dry dep to this section.

6. Page 17021, line 4: why were the concentrations initialized with 24 hr concentrations rather than mean 0 LT concentrations?

7. Page 17021, line 7: The assumption of zero background for some of the longer lived oVOCs is obviously incorrect. But perhaps it's irrelevant to the simulations here. If so, please state this explicitly. If not, perhaps aircraft observations from MILAGRO could constrain some of these values?

8. Page 17021, line 8: What does "based on the Mexico City emissions inventory" mean? The mean emissions for the region? A location in the center of Mexico City? At T0?

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9. Page 17022, top: Is there a diurnal profile on this background aerosol? Should there be? Particularly if it includes regional biogenic or fire influence? or is the temporal variability integrated over the regional background? Please detail and justify.

10. Page 17023, line 8: how is the 143 kg/km2/d value consistent with a 7.5 increase in 32 kg/km2/d given on the previous page (leading to 240 kg/km2/d)?

11. In the Figure 3 HO2 & HO2+RO2 panel: is the data for only HO2 or both? If the later, please comment on the large disagreement with the model.

12. Page 17024, line 18: note that for greater than C13 compounds the difference is over an order of magnitude.

13. Page 17025, lines 19-20: Why is afternoon SOA is so much higher than Hodzic et al?

14. Figure 7 caption (and perhaps in text): be clear that the C# refers to the C# of the precursor compound not final product.

15. Discussion of Figure 7 and in Conclusions: It should be indicated that while no validation of C14+ alkanes is available for Mexico City, given that concentrations here exceed LA measurements by over an order of magnitude, the model may significantly overestimate the SOA from this source.

16. Page 17026, line 11: The Lagrangian simulation results have not been presented yet. Section 3.4 should be moved prior to this.

17. Page 17028, line 16: to be specific “to -1 throughout the 6 days, and modeled SOA. . .”

18. Section 4.4: can you explicitly discuss the contributions from the estimate SVOC/IVOC vs. other estimated precursors?

19. Page 17038, line 3: typo “agreement”

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20. Page 17038, lines 3-5: Good agreement could also be obtained by a coincident underestimate of sources AND sinks.

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