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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 #4

Received and published: 16 August 2011

The subject manuscript by Lee-Taylor et al. reports on a chemical box model application of GECKO-A, a nearly explicit gas-phase chemical mechanism model with gas-particle partitioning. As presented in the subject manuscript, as well as in future applications, this model truly will advance the field, as the model provides insights into the gas-phase oxidation chemistry that forms condensable products in the atmosphere that can not be explored with the highly parameterized models typically used to represent ambient SOA formation. There are few, if any, other models that use this model approach, and thus it is a highly unique and valuable tool. The model approach and assumptions are clear and generally well-supported. The assessment of model performance (robust results) and sensitivity to initialization are very well described. After

addressing the minor comments below, it is suggested that the manuscript be published in ACP.

Comments: It isn't always clear, both in body and figures, whether the results/discussion refer to the Eulerian scenario, Lagrangian scenario, or both. For example, on p. 17025, line 23 starts with Figure 7 and goes into the results without specifying which results are illustrated in Fig. 7; in Figure 10, the scenario is not specified. It is suggested that the authors revise the results, discussions, and figure captions as necessary to make the scenario distinction clearer (relabeling section headers, e.g., 3.2 and 3.3, would likely help).

p. 17015, starting line 15: The cited references for formation of anthropogenic and biogenic SOA are inappropriate. Each of the cited papers has made a notable contribution to the field, but the formation of SOA from anthropogenic and biogenic precursors was pursued in much earlier work (early 90's).

p. 17023, line18: Does the overestimation of ozone tell you anything about your assumed emissions?

p. 17025, line 19: It is recommended that some suggestion(s) be made as to the general reasons for the discrepancies between the current model and the parameterized model of Hodzic et al. (2010a), given the similar treatment of emissions.

p. 17034, line 12: Are the n-alkanes used as surrogates for *all* precursors of similar volatility? Or just the unmeasured NMHCs? It seems the latter is the case. If so, suggest specifying/clarifying here.

p. 17036, starting line 24: There are also earlier more appropriate references for aqueous phase chemistry.

Line 23: Reference for early model parameterization: Odum, J. R., Hoffmann, T., Bowman, F., Collins, D., Flagan, R. C. and Seinfeld, J. H. (1996). Gas/particle partitioning and secondary organic aerosol yields. Environmental Science & Technology 30:2580-

p. 17037, line 24: The statement about the importance of C>11 n-alkanes in Mexico City seems unnecessary and largely unsupported, given the uncertainty in the emissions. It seems rather that (at least without some verification of the emissions) they represent a range of species with similar volatility/reactivity, as intended.

p. 17039, starting line 10: While the discussion of aerosol formation in the Lagrangian scenario (3.4) was interesting and likely quite important, the related conclusions do not make much sense. The authors comment that partitioning theory predicts that particles evaporate as plumes are diluted, in the absence of chemical processing, and that "quite contrarily" their model predicts continuing growth. One, the partitioning portion of the GECKO-A model employs classic partitioning theory and so partitioning theory and the GECKO-A model (at least in terms of gas-particle partitioning) are the same. Two, it is not clear what is meant by chemical processing. . .if that means gas-phase oxidation chemistry, then the statement supports the model results, as it is the continued oxidation and subsequent partitioning that produces SOA in the diluted plume. Evaporation of SOA in dilute conditions assumes that there is no gas-phase source of condensable products. In the event that there is a gas-phase source of condensable products, as in the Lagrangian application of GECKO-A, then gas-particle partitioning would predict the formation of additional SOA (as in the Lagrangian application of GECKO-A). It is suggested that this part of the conclusions be rewritten to better capture the importance of the results as presented in 3.4.

Fig. 1: Terms should be described either in a figure legend or in the caption.

Fig. 10: Suggest including the dotted red and blue lines in the legend for panel a.

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