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Atmospheric Chemistry and Physics Discussions

Interactive comment on "Evaluation of the volatility basis-set approach for the simulation of organic aerosol formation in the Mexico City metropolitan area" *by* A. P. Tsimpidi et al.

Anonymous Referee #2

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In their paper, Tsimpidi et al. present a new approach to modeling organic aerosol dynamics using 3-D atmospheric chemical transport models. As an application scenario, the authors have selected a single episode for Mexico City urban area. The paper is, in general, well written, and contains relevant scientific information that will add to the current level of understanding of organic aerosol dynamics in the atmosphere. I recommend the paper for final publication, after some issues are addressed.

General (major) comments:

An important part of the study resides in the assumptions made to construct the emissions inventory used in the modeling experiments. Additional details should be pro-

vided; at some points the description in Section 2.2 tends to be hard to follow. It would help if the authors provide a summary table indicating total domain-wide mass emissions, and the corresponding contributions from particular sources, as well as how these partition. Were all PM size bins treated equally? One would expect that the composition of ultrafine aerosols be different from coarser aerosols. Comment on the expected uncertainties from only using diesel exhaust and wood smoke data to partition the OA emissions. Are OA boundary conditions also partitioned? It is not clear.

Section 4 should be revised since it falls short on the expected level of analysis of the results from the modeling experiments; clarifications also need to be made. When discussing averages (e.g., page 13708, line 2, as well as figures), are these episode averages? 24-hour averages? If these are episode averages, comment on the logic of using this averaging scheme. Long-period averages can be misleading. Explain why only PM1 data is shown in the Figures and not more conventional PM2.5, or both. It would actually be convenient to show both to get a better understanding of fine PM behavior.

No domain-wide information is provided on diurnal/nocturnal dynamics; only time series plots at a single site is provided. Even though only one site is available for comparison, it would be of interest to look at domain-wide variations. Comment on the limitations on just having one station against which comparisons could be made.

Section 5. Be more quantitative in the conclusions derived from the time series: "reasonable agreement" is too vague. Estimate % bias, % error or other statistical measures.

Please comment on the numerical and computational burden that results from a more detail representation of organic aerosol dynamics.

Specific comments:

Page 13695, line 15 "The model predictions. . ." Awkward sentence construction.

Page 13701, line 3: Any reason why no specific VOC species were treated individually against just using lumped species?

Page 13704, line 8: How relevant is the fact that glyoxal chemistry was not treated explicitly?

Page 13703, line 12: Is this PM, PM10? How were PM emissions segregated in the different mass bins? (See first major comment)

Page 13704, line 22: Lei et al. (2007) – missing reference.

Page 13707, line 12: "OPOA is predicted to be the dominant OA component. . ." This can be misleading. From a relative stand-point the argument is correct. However it would be more convenient to indicate the absolute mass contribution to get an idea of the real importance of each component to the total mass produced. This same comment applies when discussing other relative contributions.

Figures 9 and 10. Are the authors showing episode averages hour-by-hour or is this a particular day? If the first it true, please clarify and comment on the reasons to do this.

Page 13709, line19: Should read "and".

Figure 1. "significant fraction", be more quantitative.

Figure 3. Provide coordinates along the map boundaries.

Figure 5 and 6. Use the same scale to show contributions.

Interactive comment on Atmos. Chem. Phys. Discuss., 9, 13693, 2009.