Atmos. Chem. Phys. Discuss., 9, C2931–C2934, 2009
www.atmos-chem-phys-discuss.net/9/C2931/2009/

Atmospheric Chemistry and Physics Discussions

Interactive comment on "Evaluating simulated primary anthropogenic and biomass burning organic aerosols during MILAGRO: implications for assessing treatments of secondary organic aerosols" *by* J. D. Fast et al.

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Received and published: 17 July 2009

Comment: Aromatic compounds, in particular toluene, typically serve as major SOA surrogate precursors in lumped chemistry schemes. Modeling correct concentrations of these compounds is therefore important when discussing OA. It is concluded (summary statement) that 'only predictions of aromatics were consistent with the measurements at T1'. We have observed that WRF-Chem significantly underestimates toluene mixing ratios over the city using the CAM01 and CAM04 emission inventories without adjusting these to match the more recent SMA-GDF inventory. If the modeled CO is

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'well simulated on most days and over the city' (as mentioned in the abstract), then there seems to be a significant (e.g. a factor of _2) overestimation of aromatics by the model during the day as presented in figure 18 (see average concentrations normalized by CO). It seems that conclusions drawn for VOCs would need to be discussed for a larger set of observations (maybe the comparison would look much different if data sets at T0, the G1 and the C-130 were also considered). Given these uncertainties I am not sure about the usefulness of defining TOOC in this context. It seems like comparing apples and oranges. Adding up all organic species in a lumped chemistry scheme is not the same as adding up all VOC + OA from measurements. For example there are no observational data for many intermediates produced during photo oxidation (qualitative GCxGC chromatograms have shown >500 peaks in polluted urban environments – for example Lewis et al., Nature 405, 778-781, 2000). On the other hand lumped chemistry schemes typically aim at carbon closure. So even if 'TOOC' between the lumped chemistry mechanism and observations agreed in the present case, they would most likely agree for the wrong reasons.

Response:

We removed the TOOC discussion from the revised paper, as it is not central to the main points of our work. As suggested by Dr. Karl, it would be better to present observed versus modeled TOOC comparison using other surface and aircraft measurements in addition to those at the T1 site. This will be done in a separate manuscript. Nevertheless, we will address his comments here. Dr. Karl suggests that our model results over-estimate aromatics by a factor of 2. His comment is apparently based on the assumptions that 1) toluene is the only compound included in the simulated TOOC aromatic class and 2) actual toluene emissions are much higher than the emissions inventory used in our study; thus, if our model results agree with observations we must be over-estimating toluene. The first assumption is incorrect; both the simulated and measured quantities presented for the TOOC aromatic class of compounds in our original manuscript include multiple aromatic species, not just toluene. In addressing the

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second assumption, we note that the work of Karl et al. 2009 (which we assume is the work referred to by Dr. Karl in his comment) focused on airborne flux measurements of toluene and benzene. They identified two specific areas near T0 as apparently having high toluene emissions: the Mexico City airport and an industrial area in the central part of the city. These areas are a substantial distance from the T1 ground site where the extensive field measurements conducive to the TOOC calculations we presented were made. Dr. Karl's comment that they 'have observed that WRF-Chem significantly underestimates toluene mixing ratios over the city' appears to be referring to specific grid cells in their domain located near the airport and the industrial area, as a comparison of simulated and observed values in their work was performed only for toluene, and only with C-130 aircraft measurements in that specific area. A detailed description of the model domain(s), resolution and configuration, and physics options were not identified in their paper. Nor were key performance metrics [e.g., comparisons of observed and simulated wind fields, boundary layer depths, inert and reactive chemical species concentrations, etc.] presented. We therefore cannot comment on any similarities or differences between their WRF-Chem results and ours. Additionally, using numbers from Table 2 of Karl et al. 2009, the new SMAGDF emissions inventory for the Mexico City (not available when our modeling study was initiated) show an inventory-domain-wide increase of only 18% in toluene emissions relative to the emissions inventory used in our study.

Dr. Karl also seems to be suggesting that comparisons of simulated and observed TOOC are not and never will be useful because a 1:1 match between simulated and measured quantities cannot be obtained. We respectfully disagree with this point of view. Validating model results is never easy, particularly in the case of the VOCs where models by necessity must use a reduced set of lumped/surrogate species to represent a vast number of real-world compounds. The TOOC concept is relatively new, first introduced (to our knowledge) by Heald et al. in a 2008 paper. We think it that TOOC, and the hydrocarbon categories that go into defining it, will provide a framework for at least a preliminary, quantitative analysis of model performance in simulating VOCs

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and potentially SOA, much in the same way that the concepts of NOx, NOy, and NOz provided a means to help quantify ozone modeling performance.

Interactive comment on Atmos. Chem. Phys. Discuss., 9, 4805, 2009.

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