**Atmospheric
Chemistry
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Discussions**

Interactive
Comment

Interactive comment on "Simulations of organic aerosol concentrations in Mexico City using the WRF-CHEM model during the MCMA-2006/MILAGRO campaign" *by* G. Li et al.

Anonymous Referee #1

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This study looks at the use of two different kinds of organic aerosol models in an urban setting, and investigates the possible factors contributing to the difference between modelled and observed POA and SOA concentrations. It is suitable for publication in ACP, after some modifications, as detailed below.

Pg 29350, line 9 : define MCMA the first time you use it.

Pg 29351, line 24-25: remove "..and probably play an important.......(Pope and Dockery, 2006)" since this essentially repeats what you said about aerosols in general.

Pg 29352, line 10 Write out SVOC in full when you define it. Don't combine a word and an abbreviation.

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Pg 29354, line 18: How is new particle formation parameterised in the model? This should be explained briefly (not just with a citation). New particle formation is a poorly understood process, but one which may have a substantial influence on the partitioning of SOA species, therefore the way in which the model determines the timing and magnitude of the events needs to be described.

Pg 29356, Model descriptions: Isoprene can make a significant contribution to SOA, probably even in urban areas. Is this species not included in either of the models?

Pg 29356, line 23 The organics are assumed to form a pseudo-ideal solution – How valid is this assumption? Near sources in urban environments, probably not very. There should be some discussion of the effects of solution non-ideality.

Pg 29356, line 25 : I don't understand something here. You mention that nine surrogate compounds are used for the POA components. Which components are these assumed to represent? Do you have any non-aerosol emissions in this model version? Do you include VOC?, these don't seem to be specifically mentioned here.

Pg 29357, line 14 "Robinson et al 2007"

Pg 29357, line 19 Discuss the suitability of applying this single reaction rate to all species. How is this justified?

Pg 29357, line 8 This can't be generally stated. Isoprene SOA yields for example do increase with increasing VOC/NOx ratio, but then they peak and decrease as a ratio of about 1 is exceeded. Likewise for monoterpenes although a higher VOC/nox ratio is reached before the yield decreases again. Sesquiterpenes on the other hand, form higher SOA yields as NOx values increase. See Hoyle et al. ACP 11, 321–343, 2011 for a summary.

Pg 29357, line 21: On what is the 7.5% assumption, or the shift by one volatility bin based? Is there any published evidence that shows that an oxidation reaction with OH will reduce the volatility by an order of magnitude, or add 7.5% to the mass of a

compound?

Pg 29358, line 11: Why is the sum of POA + SVOC+IVOC = 7.5POA? Is this some kind of emission scaling based on the mass of POA, or did the total just coincidently come to 7.5POA? If it is the latter, then you should re-phrase this sentence to clarify.

Section 2.3: Explain the terms "O3-convection North" and "O3-convection South". When you describe the model you must include at least a sentence describing each aspect you mention. Simply providing citations for the PBL scheme, the microphysics scheme etc. is not informative enough.

Page 29359 line 12: so it seems that you do account for isoprene emissions. You really need to list the species which are accounted for in the model description, even if they are combined into a lumped species.

Figure 2 is rather hard to interpret. It should be made clearer by making the squares showing the measurement points larger, and removing the outlines of the different regions within the city area.

Page 29361 line 18: "are contributed to the development" change to "contribute to the development".

Page 29362 line 16: You say that the night time O3 deviates from the measurements except on the 26th. I think figure 3 shows that the deviation is rather especially large during the night of the 26th. Do you have any idea what causes the over estimation in the O3 and the underestimation in CO on the night of the 26th?

Page 29362 line 17: "the complexity of the night time chemistry" What aspects of the chemistry in particular does the model have difficulties with? Please be more specific.

Page 29362 line 26: The model simulates the emissions during the day time? Aren't the emissions prescribed? Figure 4,6,8,9,10 – There are times with no data. Please state if there is a reason for this, or if the values are so low that they do not show up on the plot.

Page 29363 line 12:"...based model) diurnal" – change to :"...based model) for the diurnal"

Page 29363 line 7: "throughout the entire episode" – actually there is an overestimation until the 27th.

Page 29363 line 8: If the inventory was really missing sources, then why do you have an overestimation early in the episode? You should also mention that the 25th and 26th are Saturday and Sunday, presumably this explains some of the different pattern of emissions. The 24th on the other hand is Friday, and also shows no sign of a rush hour in panel c of figure 4.

Page 29363 line 25-page 29364 line 4: How do you get higher values of POA in the NT-SOA model than in the T2 model for the morning rush hour? POA is non volatile in the T2 model, isn't it? So there should always be more in the T2 model than in the NT model.

Page 29364 line 18 "reproduces the variability" – this is quite an over statement. The t2 model shows some squiggles which in some cases occur at the similar times to the peaks in the measurements, but just as often entirely fail to capture the changes in the measurements.

Page 29365 line 27 "two distinct peaks" I only see one peak. If there really is a second peak, it's certainly not distinct.

Page 29366 line 14-16 It is true that many of those aspects mentioned could contribute to the underestimation, however we don't really gain anything from presenting a list of the usual reasons models may not match the observations. You need to convincingly identify those aspects with the largest influence, and not just speculate on the possible causes. A few lines later you mention that the based on the CO and O3 simulation, the met fields look ok. Good, so you can already remove the meteorological fields from your list. What about the others?

Page 29367 line 17 change "Monoterpene" to "Monoterpenes"

Page 29371 line 15 change "considerably" to "slightly"

Page 29372 line 13-14 "missing background SOA transport" This statement stands a bit alone. You should mention that you look at it in more detail later.

Page 29373 line 8 The NT2E version has fixed OH levels, as I understood it, so these are not going to change as you suggest here. For the other model versions, sure.

Page 29374 line 17-18 Given the underestimation during the night and morning, I don't think aging of anthropogenic SOA is the only problem.

Page 29376 line 17-19 The agreement with observed SOA can be improved by changing these things, and some of them may contribute to the model underestimation, but you have not proved in this study that any of them were actually responsible for the model underestimation. There is a big difference in those two statements. There could well be, for example, SOA formation pathways, or precursors which one simply hasn't accounted for, which cause the majority of the underestimation.

Page 29376 line 23 change "considerably" to "slightly".

Interactive comment on Atmos. Chem. Phys. Discuss., 10, 29349, 2010.