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Geoscientific Model Development Discussions
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Interactive comment on "Modeling Regional Air Quality and Climate: Improving Organic Aerosol and Aerosol Activation Processes in WRF/Chem version 3.7.1" *by* Khairunnisa Yahya et al.

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Reply to Reviewer 2

The study is extensive, and is suitable for publication in GMD. I particularly like the summary of existing SOA approaches, centred around the VBS. This is a useful addition to the literature for sure. I request the following issues are addressed prior to publication.

Reply: We thank the Reviewer for the comments to improve the presentation of the manuscript. Where applicable, suggestions have been taken into consideration and added to the manuscript. We hope that we were able to answer all the reviewer's

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questions adequately. Please see below our point0-by-point replies.

Page 4 line 80. I'm not sure the commonly held notion of computationally expensive SOA schemes according to the number of products should persist as a general discussion. Most, if not all, SOA models assume equilibrium absorptive mass partitioning which rests on Newton based methods requiring a small number of iterations. Is there a range of % contributions, for example, that display the relative cost of SOA schemes versus, say, the gas phase chemistry?

Reply: The new SOA schemes, such as the VBS, is more computationally expensive in comparison to the "traditional" SOA schemes in 3-D models, such as the Odum 2-product model. From our experience, the SAPRC07 scheme is the most expensive compared to the other gas-phase chemistry schemes due to the number of chemical equations. Therefore, the coupled SAPRC07 with the VBS SOA model is computationally most expensive option. Unfortunately, we did not record the actual computational cost for each of the SOA schemes or the gas-phase chemistry schemes.

The end of section 1.2 Would it be possible for the authors to comment on what conditions the activation schemes are initialised? Running at higher than 1km, presumably the assumption is to use the aerosol composition, both SOA and SIA, at a speciïňĄc RH which is then fed into the ARG or FN schemes with regards to hygroscopicity? This might also impact the performance of any given activation scheme if the assumed mass is from a 'dry' SOA partitioning model, whereas SIA accounts for RH dependent partitioning.

Reply: The chemical initial and boundary conditions (ICONs/BCONs) come from the modified CESM/CAM version 5.3 with updates by Gantt et al. (2014), He and Zhang (2014), and Glotfelty et al. (2016). Only the SIA concentrations are present as ICONs/BCONs. A 10-day spin-up is also used for the SOA concentrations to stabilize.

Section 3.1: How does the new treatment of semi-volatile POA work with boundary

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conditions used to initialise simulations? What is the impact of forcing different VBS proïňĄles into one? I wasn't clear how this relates to, for example, the inputs required for the CCN schemes. Is it related to an inability to track separate sources through the simulation? Or is it related to how the emissions are convolved?

Reply: As mentioned above, other than the differences in POA emissions as mentioned in the text, there are no other differences in ICONs/BCONs used in all the VBS cases. The model is unable to track the use of different VBS profiles in 1 simulation. Different simulations would have to be run, each changing 1 parameter to understand how the particular change affects SOA concentrations and CCN. The standard model inputs apply for both the VBS schemes, and the CCN schemes. No other special model inputs are required to run the CCN scheme, as the CCN scheme is dependent on the aerosol concentrations from the chemistry schemes, and vice versa.

Section 4.3 Related to a previous point, the authors comment on how larger differences in CDNC predictions arise from different gas-phase mechanisms over VBS variants. I think it would beneïňĄt the reader, and the context of the sensitivity simulations to comment on how the VBS versus RH interactions feed into the CDNC parametrisations.

Reply: The evaluation of the performance of RH by the model is interesting but beyond the scope of this study. However, from previous research, for example, by Yahya et al. (2015, 2016), the model performs relatively well for RH. We also do not expect RH to vary much between the different VBS cases. To ultimately understand how RH impacts the VBS performance, we would have to artificially vary the RH as inputs to the model. This might work better as a box-model study, rather than for a 3d model, where RH is predicted, and is temporally and spatially varying.

References: Yahya, K., J. He, and Y. Zhang (2015), Multiyear applications of WRF/Chem over continental U.S.: Model evaluation, variation trend, and impacts of boundary conditions, J. Geophys. Res. Atmos., 120, 12748–12777, doi:10.1002/2015JD023819.

Yahya, K., Wang, K., Campbell, P., Glotfelty, T., He, J., and Zhang, Y.: Decadal evaluation of regional climate, air quality and their interactions over the continental US using WRF/Chem version 3.6.1, Geosci. Model Dev., 9, 671 – 695, doi:10.5194/gmd-9-671-2016, 2016

A more philosophical question, which doesn't require any modiïňĄcations and isn't a critique of this study: I often wonder how much value we should place on assuming accurate ambient OA/OC measurements without going back to trailing the same model permutations in a controlled environment. Would the authors value smog chamber studies, on mixed VOC systems, using the same parametrisations but in a box-model conïňĄguration? It seems that, at least, this would be valuable from a high accuracy measurements perspective.

Reply: Smog chamber studies, as well as box-model configurations are definitely valuable. In our opinion, they offer complementary information to 3-D model testing. As a matter of fact, many smog chamber and box-model studies were indeed carried out first, before the incorporation of the derived parameterisations into a 3-D model such as the WRF/Chem model in this study. While box model studies are confined to a controlled environment, using the 3-D model in our case represents real atmosphere yet it introduces other uncertainties to OA concentrations from other atmospheric variables, feedbacks and processes. Both smog chamber studies/box-model studies and 3-D model studies have their own purposes and strengths, and should be used when resources are permitted.

Minor comments: Abstract line 41:'to 7.1%, it, however'. Please break the sentence here

Reply: This has been modified.

page 14 line 316-317:'based on a number of literature', should be 'based on a number of studies in the literature'

Reply: This has been modified.

page 29, lines 661-662:'simulated vs, observed' please replace this with 'simulated versus observed'

Reply: This has been modified.

Please also note the supplement to this comment:
http://www.geosci-model-dev-discuss.net/gmd-2016-288/gmd-2016-288-AC2-supplement.pdf

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