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Interactive comment on "Two new submodels for the Modular Earth Submodel System (MESSy): New Aerosol Nucleation (NAN) and small ions (IONS) version 1.0" *by* Sebastian Ehrhart et al.

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AR: We thank Referee 2 for their time and for the useful suggestions and correction. Here we addressed all comments (reporting the original comments). The manuscript has been improved accordingly.

Printer-friendly version

Discussion paper

General comments:

RC: In the manuscript the authors introduce two new sub-modules into the EMAC/MESSy framework for calculation of new particle formation. NAN calculates nucleation via several pathways and is largely based on experimental results of CLOUD chamber experiments, published previously. Since the new parameterization of nucleation in the NAN depends on atmospheric ions, these were also introduced in MESSy as sub-module IONS. Although most of the previous CLOUD studies also introduced their new process parameterizations (eg. ion induced ternary nucleation, nucleation involving oxidized organics and pure organic nucleation) into global aerosol models, the coupling with a global chemistry model was not realized yet. Thus, further studies with EMAC/MESSy could also evaluate chemical factors. Moreover, NAN includes several nucleation pathways involving also stabilizing ammonia/ amines and oxidized organics, both neutral and ionic. This approach might be very promising regarding to future usage disentangling dominant pathways as for polluted and pristine environments. In general, the manuscript is structured well and clearly written. Thus, I recommend to accept the manuscript for publication after some minor corrections and clarifications I address in my comments below.

AR: We thank the referee for the positive comments on the manuscript. Further studies utilising the new submodels and improved reactions will certainly be conducted and looked at these topics in more detail.

Specific comments:

RC: On page 8 you describe the simulations done for testing and evaluating the new sub-modules. Table 2 shows the overview over the model runs, four runs appear there. GMXe, the base run including the new paramterization Dunne et al. (2016) within

GMXe, Dunne 1 and Dunne 2 (same parameterization, but calling the sub-module before and after GMXe) and a run named Organic. What is the difference between Dunne 2 and Organic? In the results section, page 10 and 11 the run Organic is not mentioned and not shown in any figure. Please clarify in the text.

AR: We assume the referee meant Table 1, based on the text of their comment. The run labelled organic is shown in Figure 7 and 8. The organic nucleation was not implemented in GMXe and the effects of calling nucleation outside of GMXe was tested only with the inorganic nucleation, as H_2SO_4 and NH_3 are already part of GMXe. We removed the organic entry from Table 1 to avoid this confusion.

RC: In pages 6, 7 and 8 you mention different (or not different?) HOMs. Please clarify the difference between HOM, HOMOH, HOMO3, HOMOOH, HOMOO3.

AR: $HOMO_{OH}$ and $HOMO_{O_3}$ are typos. We corrected them in the revised version of the manuscript. HOM_{OH} are products of monoterpene oxidation by OH radicals that can nucleate. HOM_{O_3} are products of monoterpene oxidation by O_3. HOM without any subscript is the sum of HOM_{OH} and HOM_{O_3} (page 7, line 2 of the original discussion paper).

RC: HOMs were not inlcuded in ORACLE and added for this study. How does ORACLE treat these HOMs?

AR: Species that form SOA can be added to ORACLE via namelists. The chemistry of HOM_{O_3} and HOM_{OH} formation is described in R6 and R7, this reaction was added to the ORACLE chemistry as described in Tsimpidi et al. (2014). These HOMs are then added to an ORACLE volatility bin and treated in the same way as other species in ORACLE according to their vapour pressure (page 8 line2 31-32).

RC: Do they also undergo SOA formation driven by ORACLE, outside of nucleation

events? How do they interact with pre-existing aerosol?

AR: If aerosol particles are present, HOMs will be partitioned between gas phase and particle phase by ORACLE.

RC: How much SOA formation results from taking into account the improved nucleation in MESSy? You mentioned the study by Tröstl et al. 2016, where they describe accelerated particle growth due to low and semi volatiles, which are simulated and used in ORACLE. On page 7 you describe the total nucleation rate and you show particle numbers in the results section. Nevertheless, as you consider various new particle formation pathways, I wounder if you already identified (maybe regionally and temporally) dominant pathways? This would be an interesting point for discussion about competing processes.

AR: The aforementioned questions will be subject of more detailed studies with these new submodels.

Technical corrections:

RC: Page 5, line 1: change "The radius of the aerosol particles is provide“ to "... is provided“.

AR: We corrected this.

RC: Page 6, line 10: the first "in“ is redundant.

AR: We corrected the sentence.

RC: Page 6, line 12: change "oni“ to "on“.

AR: We fixed this mistake.

RC: Page 9 Table 1: In the caption you describe "Position“, but in the table the header is "NAN called“, please clarify.

AR: We corrected the header. It is now in accordance with the text "Position".

RC: Page 19, Table 2: Change "altitude“ to "Altitude“ for consistency.

AR: We changed the text and also added the information that altitude is in m.

RC: Page 25, Figure 6: The caption is wrong according to the run Dunne 2, please change "just before“ to "after“.

AC: We corrected the sentence.

References

Tsimpidi, A. P., Karydis, V. A., Pozzer, A., Pandis, S. N., and Lelieveld, J.: ORACLE (v1.0): module to simulate the organic aerosol composition and evolution in the atmosphere, Geoscientific Model Development, 7, 3153–3172, doi:10.5194/gmd-7-3153-2014, http://www.geosci-model-dev.net/7/3153/2014/, 2014.

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