

## **Review of the manuscript „Two new submodels for the Modular Earth Submodel System (MESSy): New Aerosol Nucleation (NAN) and small ions (IONS) version 1.0“**

### **General comments:**

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.

### **Specific comments:**

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 parameterization 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.

In pages 6, 7 and 8 you mention different (or not different?) HOMs. Please clarify the difference between HOM, HOM<sub>OH</sub>, HOM<sub>O<sub>3</sub></sub>, HOMO<sub>OH</sub>, HOMO<sub>O<sub>3</sub></sub>.

HOMs were not included in ORACLE and added for this study. How does ORACLE treat these HOMs? Do they also undergo SOA formation driven by ORACLE, outside of nucleation events? How do they interact with pre-existing aerosol?

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 wonder if you already identified (maybe regionally and temporally) dominant pathways? This would be an interesting point for discussion about competing processes.

**Technical corrections:**

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

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

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

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

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

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