

Interactive comment on “The MESSy aerosol submodel MADE3 (v2.0b): description and a box model test” by J. C. Kaiser et al.

Anonymous Referee #1

Received and published: 10 February 2014

The manuscript describes development of the MADE3 aerosol module to treat interactions of coarse particle components with gas-phase species and other particles. The partitioning of total chloride between the gas and particle phases is also incorporated into MADE3. The MADE3 aerosol module is then tested for a boxmodel scenario under idealized conditions representing shipping emissions in the marine boundary layer. The PartMC-MOSAIC model is run for the same boxmodel scenario and is used as a reference to benchmark the results of the simpler MADE3 model. Overall, this is a worthwhile study, and I commend the authors on their efforts to test their aerosol module in stand-alone mode, where it is easier to isolate issues than in the 3D simulations with chemical transport models.

General Comments:

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1. The authors report large deviations in number size distributions predicted by MADE3 and PartMC-MOSAIC in the diameter range critical for CCN activation and conclude that, “We will therefore have to be careful when interpreting CCN calculations in 3-D model applications.” This conclusion should be revised. If the deviations found here are likely to have a large impact on CCN concentrations, then further model development would be required for applications involving CCN. The authors should also indicate if the large deviations seen here are an artifact of the boxmodel approach (where transport, deposition, etc. are not included) and if these differences would likely be smaller in a 3D application.

2. The Appendix compares size-composition distributions for MADE3 and PartMC-MOSAIC at the end of the simulation period, and the authors conclude that there is broad agreement between the models. However, Figure A.1 appears to show some important differences. BC concentrations are elevated at small diameters in PartMC, and PartMC shows a decreasing trend in sulfate concentration with increasing diameter for fine particles. This behavior, which seems reasonable, is not captured by MADE3, but could potentially be important in many applications. The authors should do a better job of discussing differences in size-composition distributions, even if it is difficult to perform a perfect 1-to-1 comparison between these models.

3. In several places in the manuscript, the use of different thermodynamic modules in MADE3 and PartMC-MOSAIC complicates the interpretation of differences in model predictions. If the authors were to re-run the test case using the MOSAIC thermodynamic module within the MADE3 formulation, it would help separate differences in model predictions that are due to aerosol dynamics and thermodynamics.

4. The authors considered only one boxmodel test case (marine conditions) because their initial 3D application will focus on shipping impacts. However, MADE3 will likely be applied under diverse conditions in the future. Including additional test cases (e.g., mixing of urban and marine air masses near the coast) could also be informative.

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Specific comments:

–Abstract: Please clarify that the model described here is MADE3v2.0b (if that is the correct version). There could be confusion because the article appears to describe the beta version of version 2 of the 3rd generation of the MADE model.

–Abstract, line 23: Please clarify that “total aerosol composition” is being referred to (size-composition distributions appear to differ significantly between the models).

–Section 2.1.2: Please clarify if H₂SO₄ can condense onto insoluble BC/Dust distributions

–p. 701, line 21: In this manuscript, is “coarse particles” used to indicate the large diameter modes?

–p. 701, line 27: You should probably add the Sun and Wexler (1998, AE) reference for completeness

–p. 702: Please clarify why H₂SO₄ is being treated dynamically when the previous page indicates that time scales justify an equilibrium approach and equilibrium is assumed for other components. Is this related to the need to treat nucleation for H₂SO₄?

–p. 711, line 24: The phrase “coarse particle interactions” is used in various places in the article. Please clarify what is meant in the context of marine conditions. For example, is the issue water competition during activation, effects of giant CCN on autoconversion, etc.? Also, the manuscript seems to imply that the replacement of Cl by NO₃ could be important for water uptake and activation. Is this so? I would think that soluble coarse particles would easily activate regardless of whether they contained NaNO₃ or NaCl.

–p. 712: It might be helpful to include a table of initial conditions for the model simulations in case other groups would like to repeat the test with their models.

–p. 717, line 18: As the authors are probably aware, it is possible to simulate the evolu-

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tion of particle mode standard deviations dynamically. Models such as CMAQ currently do this, although they include limits on the range in which the standard deviations can vary, and so it is unclear how numerically stable these calculations are.

–p. 719, lines 9-10: Does this mean that coarse particles components were effectively in equilibrium with the gas phase in MADE3 in this test case?

Interactive comment on Geosci. Model Dev. Discuss., 7, 691, 2014.

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