

Interactive comment on “A detailed aerosol mixing state model for investigating interactions between mixing state, semivolatile partitioning, and coagulation” by J. Lu and F. M. Bowman

Anonymous Referee #2

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The authors present a detailed description of the Detailed Aerosol Mixing State (DAMS) method for representing the evolution of aerosol populations comprised of multiple compositional populations. Using an idealised five-component system it investigates the combined influences of representation of mixing state and condensation/coagulation on the modelled aerosol mass and number distributions.

It is, on the whole, a well written and detailed description of the DAMS method, and a good analysis of the behaviour of the aerosol populations in different modelling regimes. I agree, however, with Referee 1 that the paper would be improved with a more detailed model description, and that an extra figure showing the mass distribu-

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tions of the populations shown in Figure 4 and Table 3 would be helpful. I also would like to see more discussion of computational costs and how changing the mixing criterion changes these (more details in the specific comments below). Overall I think the paper fits well into the scope of ACP, and recommend it for publication.

Specific Comments:

1) The externally-mixed five-component scheme used as an example in this paper consists, with the DAMS method, of 31 different mixture populations. 9 populations are described as significant for the base case with a mixing criteria of 0.1, with only an extra 5 populations considered when examining the effects of changing the mixing criteria. This raises two questions, one on computational costs, the other on the choice of mixing criteria.

1a) What is the computational cost of the externally-mixed scheme compared to the internally-mixed scheme? Is it dependent on the number of populations present? And if so how does this cost change with the choice of mixing criteria (and so number of major, and minor, populations)?

1b) Choosing a mixing criteria which is based on the mass fractions of the individual components makes sense when we have no *a priori* knowledge of the probable aerosol mixing state. However, for systems where there are distinct populations of components which we know are likely to be found together in the condensed phase, then surely it makes more sense to build the mixing criteria around the populations of components rather than the individual components. For example, in this paper there are three obvious component populations: INERT, POLAR (PO2 and SV2) and NON-POLAR (PO1 and SV1). Basing the mixing criteria on these component populations would reduce the number of separate mixture populations to 7, all of which would major populations, with only a little information lost (populations 4b, 7 and 7a from Table 4 would be combined, with probably a small percentage the mass of each ending up in populations 4, 5 and 6), and probably with a large saving in computational costs. Atmospheric sys-

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tems are more complex than this, but enough component groupings exist that such an adaptation of the model would be worthwhile. Does your model have the flexibility to change the basis of the mixing criteria in this manner? If so then it would be informative to see the effects of such a change in mixing criteria on the aerosol distributions. If not then can you state if you intend to add this functionality to the model or not?

Technical Comments:

- 1) Equation 4: this would be clearer if radius (R_{pj}) was used rather than diameter (D_{pj}).
- 2) Page 423 (and elsewhere): usage of compound/component could be made more consistent.
- 3) Page 433, line 14: "Tabl" should "Table".

Interactive comment on Atmos. Chem. Phys. Discuss., 10, 417, 2010.