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Atmospheric Chemistry and Physics Discussions

Interactive comment on "Atmospheric Cluster Dynamics Code: a flexible method for solution of the birth-death equations" *by* M. J. McGrath et al.

Anonymous Referee #2

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This manuscript describes a computer code developed to study new particle formation in the atmosphere. The work appears to be sound and well explained, and the use of a computer scripting language to generate the equations solved is novel. However, in my view the results presented are of only limited significance, constituting a somewhat preliminary report on the abilities of the code.

Key assumptions of the work are that clusters containing more than 4 acid and/or base molecules leave the system never to return, and that such clusters are formed by colliding clusters containing at least one acid molecule. Neither of these assumptions appears to be well-substantiated and although the authors note that formation rates

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may be “artificially overestimated,” they do not discuss to what extent the behaviour they observe in their results may be artefacts of these assumptions. In single component nucleation it is essential to include clusters of the critical size in any simulation and I would expect something similar in the two component case considered in here (although the definition of “critical size” may be less clear). What steps have the authors taken to ensure that they are not just looking at subcritical clusters?

The authors find that cluster concentrations vary strongly with temperature and sticking probability. The strong dependence on temperature is well known and not particularly surprising, since (as noted by the authors) the evaporation coefficients are strongly temperature dependent. On the other hand, the variation with sticking probability needs more discussion. The authors attribute the large effect to the “highly non-linear behaviour” of the system and promise to examine this effect in more detail in future, but a more specific cause should be given in the present work. It should be noted that for single component nucleation, changing the sticking probability has only a limited effect on nucleation rates, since reducing collision coefficients also reduces the evaporation coefficients when the detailed balance condition, eq. (3), is used to determine the latter.

The colour contour plots look somewhat monochromatic to my eyes, mostly appearing varying shades of blue, with some violet and red regions. I am not sure if this is a feature of the plotting software used, but I would find them clearer if there were a wider range of colours (e.g. also green, orange and yellow) in the plots.

I would suggest omitting section 2.2 on ionic clusters as only preliminary results for these are presented in the paper- I think it would be better to include this section in the promised future work examining ionic clusters in more detail.

Interactive comment on Atmos. Chem. Phys. Discuss., 11, 25263, 2011.

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