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Interactive comment on "A computationally efficient inorganic atmospheric aerosol phase equilibrium model (UHAERO)" *by* N. R. Amundson et al.

Anonymous Referee #1

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Referee comment on "A computationally efficient inorganic atmospheric aerosol phase equilibrium model (UHAERO)" by N. R. Amundson, et al.

The work presented by Amundson et al., presents a new thermodynamic inorganic gas-aerosol equilibrium model, named UHAERO, that is claimed to be both computational efficient and rigorous, as it is designed to compute deliquescence and crystallization behavior without any a priori specification of the relative humidity of deliquescence or crystallization. The latter aspect is new, but its applicability questionable.

The authors lack to provide the reader with results that are convincing that the title is

justified. To be convincing the authors should present a comparison with other widely used thermodynamic inorganic gas-aerosol equilibrium models. Disturbingly the authors did not even mention the one, which was designed for computationally efficiency. Instead, only complicated phase diagrams and a new but questionable (due to the lack of thermodynamical data on e.g. the molecular volume of the salts of interest) theoretical derivation is presented. There is further no discussion of the uncertainty to the assumptions and to my opinion the paper could benefit from a proper sensitivity analysis. A further real drawback, in the light of the current state-of-the-science is the lack of discussion of the applicability and the extension to mixed inorganic/organic aerosol systems, which are most important for a model application to reality.

I recommend publication at ACP only, if the authors have improved the manuscript by taking the following points into account, i.e.:

1. The manuscript needs to be updated to include references of all relevant thermodynamic gas-aerosol equilibrium models, including the one that was especially designed to be computational efficient, i.e. Metzger, S. M., F. J. Dentener, J. Lelieveld, and S. N. Pandis, Gas/aerosol partitioning I: A computationally efficient model, J Geophys. Res., 107, D16, 10.1029/2001JD001102, 2002. Table 1 needs to be updated. (see e.g. Table 1 presented in Trebs, et al., J Geophys. Res., 110, D07303, doi:10.1029/2004JD005478, 2005).

2. An uncertainty analysis needs to be included for the assumption on the thermodynamic data (e.g. missing molecular volume of the major inorganic salts and surface tensions) and the sensitivity of the phase partitioning to e.g. the expectation times, temperature, etc.

3. A comparison of the phase partitioning by UHAERO with those computed with the widely used thermodynamic models SCAPE2 and ISORROPIA (both are available and cited in the manuscript). This comparison should include the hysteresis loop (similar to Fig 3, 5, 7, 9, 11) for various inorganic aerosol systems (DRHs for single solute

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and multicomponent solutions, also referred to in the literature to the above models as RHDs and MDRHs, respectively). Differences should be discussed.

4. Also, a comparison for the computational burden (CPU time) should be included for the computations (and comparison) of point 3, by using the same computer systems for the computations. Such a comparison is essential in order to justify whether the proposed model is really computationally efficient enough for incorporation into regional or global atmospheric models - something that is suggested/implied by the title. If the model does not hold what the title suggests, the title needs to be changed to exclude "computationally efficient" as this would be misleading for the modeling community.

5. Further, the discussion needs to be extended to cover the overall uncertainties of the phase partitioning with respect to the inorganic aerosol systems presented. Additionally, the applicability and the possibility for extension to mixed inorganic/organic aerosol systems should be discussed.

Interactive comment on Atmos. Chem. Phys. Discuss., 5, 9291, 2005.