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Atmospheric Chemistry and Physics Discussions

Interactive comment on "Identification of molecular cluster evaporation rates, cluster formation enthalpies and entropies by Monte Carlo method" *by* Anna Shcherbacheva et al.

Anonymous Referee #2

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1. The author proposes to use the Markov chain Monte Carlo (MCMC) algorithm to solve the problem of cluster evaporation rate based on cluster distribution, and this is a novel idea for us to evaluate the thermal stability of clusters. But I have a question about the cluster distribution. The author uses ACDC to simulate the cluster distribution (from 1SA.1NH3 to 5SA.5NH3 box) instead of experimental data. Is this simulation result good enough to replace the experimental data? Simulation results are affected by accurate structure, calculation method and basis set. So I suggest that first the author expand the SA.NH3 system to a larger size (1.7 nm). Before using MCMC, simulate the SA.NH3 formation rate and compare it with the experiment data (Nature 502, 359-363, 2013) to illustrate the reliability of the simulation cluster distribution.

2. "time-independent steady-state" in abstract could be revised to be "steady-state";

3. The motivation and test results about the case of single temperature steady-state cluster distributions should be mentioned in the abstract;

4. The best result in this study is the case for steady-state concentration with two temperatures. Is this conclusion general or very specific? How sensitive towards the number of ammonia concentrations and the box size (referring to the cluster types here) is this conclusion?

5. VODE mentioned in L107 may be different from the solver used in McGrath et al. (2012) (ode15s). If so, "A detailed description of this program was published in McGrath et al. (2012)." should be deleted and a simple benchmark should be made to compare different solvers.

6. For table 3, why the minimal values of H and S are set to be -400?

7. L156, "ACDC plus VODE" should be revised to be "ACDC based on VODE";

8. L233, "upper limit" needs to be explained further.

9. L244, "well-defined" need to be defined.

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