The manuscript by Shen et al. presents simulations of new particle formation from sulfuric acid (H_2SO_4) and dimethylamine (DMA) by molecular cluster kinetics modeling. The thorough comparisons of formation rates obtained with different thermochemistry input data sets and kinetic model assumptions provide very useful information on variations and uncertainties in predicted formation rates.

I would like to bring up previous works applying ACDC-based particle formation rate look-up tables in large-scale 3D modeling, as the authors may not be aware of them (e.g. L118-119). These previous studies have applied look-up tables in the PMCAMx-UF, GEOS-Chem-TOMAS and EC-Earth3 chemical transport or Earth system models with the following particle formation mechanisms:

- H_2SO_4–NH_3–H_2O with electrically neutral clusters (Baranizadeh et al., 2016; Croft et al., 2016),
- H_2SO_4–NH_3–H_2O + H_2SO_4–DMA with neutral clusters (Julin et al., 2018; Olin et al., 2022), and
- H_2SO_4–NH_3 including both neutral and ionic species (Svenhag et al., 2024).

Most of these studies applied quantum chemistry data corresponding to the RICC2 method, as those were the only available complete data sets at the time. A comparison of global H_2SO_4–NH_3 particle formation and its effects as predicted by either DLPNO or RICC2 is presented by Svenhag et al. (2024). While DLPNO is the current best available method, it may underpredict formation rates under certain conditions (e.g. Besel et al., 2020), and the DLPNO-based rates were thus applied to assess the lower limits of the predicted effects.

In the first studies, the calculation and interpolation of look-up tables were hard-coded for the given chemical components. The most recent work (Svenhag et al., 2024) applies automatized look-up table generator and interpolator that are applicable to arbitrary components (Yazgi and Olenius, 2023), enabling easy incorporation of tables obtained for different species and thermochemistry data. Automatization is needed especially for reading in and interpolating tables within the 3D model, as it is not feasible to maintain separate interpolation routines for different tables, corresponding to different chemical mechanisms and/or dimensions.

It can also be noted that the usage of pre-calculated formation rates (which is necessary in computationally heavy 3D models) involves simplifying assumptions on gas–particle kinetics, as there are no explicit interactions between the clusters and the nucleating vapors and larger nanoparticles. Therefore, a parameterization or look-up table approach may give biased results under some conditions even if the thermochemistry data were perfectly accurate. In computationally light-weight models, this can be circumvented by explicit simulation of the coupled gas–cluster–aerosol system (Olenius and Roldin, 2022), corresponding to a multi-component adaptation of discrete–sectional modeling (Li and Cai, 2020).

Finally, I also encourage to refer to the ACDC code repository (https://github.com/tolenius/ACDC) in order to provide a reference for the model tools for reproducibility of simulation results.

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