Contribution ID: **4** Type: **not specified**

Tackling the chemical complexity of atmospheric particle formation by molecular level models

Tuesday 7 May 2024 13:45 (30 minutes)

Roughly half of the atmospheric particles originate gas-to-new-particle conversion which was first observed in the1990s. However, the molecular mechanisms of formation of the initial molecular clusters and their growth to atmospheric aerosol particles in the diverse atmospheric conditions are not yet understood. Our cluster population dynamics model (ACDC, first published in 2012) combined with high-level quantum chemical data can fairly accurately predict new particle formation rates for any single combination of clustering molecules. The sheer number of potential - predominantly organic - chemical species, processes and cluster structures makes a brute-force application of such a model impossible for most conditions in the real atmosphere. The low concentrations of the individual particle-forming vapours and their precursors, furthermore, pose challenges to their experimental identification. We have set out to tackle these issues by developing tailor made machine learning techniques to model atmospheric particle formation, and also support the analysis of experimental data

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