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Modelling of externally mixed particles in the atmosphere

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Particles present in the atmosphere have significant impacts on climate as well as on human health. Thus, it is important to accurately simulate and forecast their concentrations. Most commonly used air quality models assume that particles are internally mixed, largely for computational reasons. However, this assumption is disproved by measurements, especially close to sources. In fact, the externally-mixed properties of particles are important for aerosol source identification, radiative effects and particle evolution. In this study, a new size-composition resolved aerosol model is developed. It can solve the aerosol dynamic evolution for external mixtures taking into account the processes of coagulation, condensation and nucleation. Both the size of particles and the mass fraction of each chemical compound are discretized. For a given particle size, particles of different chemical composition may co-exist. Aerosol dynamics is solved in each grid cell by splitting coagulation and condensation/evaporation-nucleation processes. For the condensation/evaporation, surface equilibrium between gas and aerosol is calculated based on ISORROPIA and the newly developed H^2O (Hydrophilic/Hydrophobic Organic) Model. Because size and chemical composition sections evolve during condensation/evaporation, concentrations need to be redistributed on fixed sections after condensation/evaporation to be able to use the model in 3 dimensions. This is done based on the numerical scheme HEMEN, which was initially developed for size redistribution. Chemical components can be grouped into several aggregates to reduce computational cost. The 0D model is validated by comparison to results obtained for internally mixed particles and the effect of mixing is investigated for up to 31 species and 4 aggregates. The model will be integrated into the air quality modeling platform POLYPHEMUS to investigate its performance in modeling air quality by comparing with observations during the MEGAPOLI (Megacities: Emissions, urban, regional and Global Atmospheric POLlution and climate effects, and Integrated tools for assessment and mitigation) campaign in July 2009.