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A Microphysical and Chemical Model with Internally Mixed Representation: Eulerian versus Lagrangian Approach

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The accurate and efficient description of aerosol microphysical and chemical processes is required for the assessment of radiative and chemical effects of natural and anthropogenic atmospheric aerosols. The combined modeling of microphysical and chemical processes in the gas and aqueous phase such as meteorological changes, transformation of chemical species in the gas and liquid phase and the transfer of species from one phase to the other is required. Since the aforementioned processes proceed on similar time scales the usual time splitting schemes which perform process by process in a sequential order are not appropriate. In contrast to other approaches where a microphysical and a cloud chemistry model are coupled the new approach treats both processes in a unified way both from the modeling and numerical point of view. It is argued that this new model type is better suited for incorporation in multidimensional atmospheric and transport models. Essential parts of the model are outlined. The differential equations are discretized in mass space by a discontinuous Galerkin method and integrated after that in time by an implicit-explicit time integration scheme.

If coagulation plays no role the model can be run in an Eulerian fixed grid or a moving bin (Lagrangian) mode. The Eulerian fixed grid approach is compared with a 2000 bin moving simulation to demonstrate the merits and disadvantages of fixed grid for an air parcel flow over a hill. The appearance of a bimodal structure in the particle number distribution caused by numerical diffusion and/or chemical processing is discussed. Different fixed grids which differ in the number of bins and the distribution of the bins are analyzed. Furthermore the number of activated particles and the gas uptake for the different model configurations are compared.