MODELLING OF TROPOSPHERIC MULTIPHASE PROCESSES: FIRST RESULTS OF THE AFO2000-RESEARCH PROJECT MODMEP

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The complexities of cloud processes have often discouraged investigators from simultaneously treating all aspects of multiphase chemistry and microphysics with equal rigor. The description of cloud processes in the currently available box models and Eulerian grid models (cloud or mesoscale models) focuses either on detailed microphysics or complex multiphase chemistry. The chemical conversions in the liquid phase are described only in a few aggregated drop classes, or strongly simplified chemical mechanisms are used. The objective of the present project is the development of a cloud module which combines a complex multiphase chemistry with detailed microphysics. The description of both components is given for a fine-resolved drop spectrum. An efficient numerical solution of the entire complex model strongly requires the development of new numerical methods. In the framework of the joint project, techniques will be provided and tested which allow the description of complex multiphase chemistry and of detailed microphysics in multidimensional chemistry-transport models. The development is performed in close cooperation with the joint cloud experiment project FEBUKO (Herrmann et al.).

The extension of the chemical mechanism will focus on a better description of the oxidation of dissolved organic compounds within aqueous particles. For higher organics which may partition from the gas phase, phase transfer will be described by gas phase diffusion, mass accommodation and Henry solubility. Another objective consists in the development and the application of an automated method of analysis and reduction for multiphase reaction mechanisms. This leads to the derivation of reduced mechanisms for specifiable application purposes. The fine resolution of the drop spectrum used in the microphysical cloud model will be extended to the treatment of detailed multiphase chemistry. The aqueous phase concentrations are coupled both via the gas phase and via the liquid water transfer (coalescence, drop disintegration). It is investigated whether and which processes can be integrated decoupled with which loss of exactness and which gain of efficiency. A major task is the development of implicit time integration methods which integrate all involved processes in a coupled manner. This includes a.o. the development and the test of solution methods for large, sparse, linear equation systems. An efficient solution of such systems is only possible utilizing the special structure.