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Treatment of non-ideality in the multiphase model SPACCIM

R. Wolke, J. Zoboki, A. Tilgner, H. Herrmann
Leibniz-Institut für Troposphärenforschung, Leipzig, Germany (wolke@tropos.de)

The air parcel model SPACCIM ("Spectral Aerosol Cloud Chemistry Interaction Model") was developed for the description of cloud processes which combines a complex multiphase chemistry with detailed microphysics (Wolke et al., 2005). The description of both components is given for a fine-resolved particle/drop spectrum. Depending on the used microphysical model, external and internal mixing of aerosol populations can be taken into account. The activation of droplets is explicitly described. Changes of the chemical aerosol composition by gas scavenging and chemical reactions feed back on the microphysical processes (e.g., water condensation growth rates via changes in the Raoult term). The model allows a detailed description of the evolution of gases and particles before cloud formation, during the cloud life time and after cloud evaporation. The performance of the model was shown for simple chemical mechanisms (with only inorganic chemistry) as well as for very complex mechanisms of the CAPRAM (*http://projects.tropos.de:8088/capram*) family which contain a detailed description of the organic chemistry. The model is evaluated with data from the FEBUKO field campaign (Tilgner et al., 2005).

In the published SPACCIM version, well-diluted droplets are assumed. In fact, the assumption of an ideal solution is not valid especially for non-activated particles and small droplets. The non-ideal behaviour can be described by activity coefficients. In the past, thermodynamic models have been developed to predict the equilibrium composition of water-organic-electrolyte aerosols (e.g. Clegg et al., 2001; Ming and Russell, 2002). These approaches are based upon the combination of existing models of inorganic electrolyte solutions and water-organic mixtures. For the determination of activity coefficients, an extended version of UNIFAC (e.g., Raatikainen and Laaksonen, 2005) coupled with the Pitzer method (e.g., Clegg and Pitzer, 1992) is implemented in SPACCIM. The used approach and first results are presented in the paper. For the model studies, a complex multiphase reaction scheme extracted from CAPRAM is applied. The effects of non-ideality are discussed for a test scenario with three cloud cycles.

References

Clegg, S.L., Pitzer, K.S., 1992. Thermodynamics of multicomponent, miscible, ionic solutions: Generalized equations for symmetrical electrolytes. Journal of Physical Chemistry, 96, 3513-3520.

Clegg, S.L., Seinfeld, J.H., Brimblecombe, P., 2001. Thermodynamic modelling of aqueous aerosols containing electrolytes and dissolved organic compounds. Aerosol Science, 32, 713-738.

Ming, Y., Russell, L.M., 2004. Organic aerosol effects on fog droplet spectra. Journal Geophysical Research – Atmospheres, 1009.

Raatikainen, T., Laaksonen, A., 2005. Application of several activity coefficient models to water-organic-electrolyte aerosols of atmospheric interest. Atmospheric Chemistry and Physics Discussions, 5, 3641-3699.

Tilgner, A., Majdik, Z., Sehili, A.M., Simmel, M., Wolke, R., Herrmann, H., 2005. SPACCIM: Simulations of the multiphase chemistry occurring in the FEBUKO hill cap cloud experiments. Atmospheric Environment, 39 (23-24), 4389-4401.

Wolke, R., Sehili, A.M., Simmel, M., Knoth, O., Tilgner, A., Herrmann, H., 2005. SPACCIM: A parcel model with detailed microphysics and complex multiphase chemistry. Atmospheric Environment, 39 (23-24), 4375-4388.