



## Scalable kinetics treatment for gas–aerosol systems in atmospheric models

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As computational capacity increases, large-scale atmospheric models are able to handle more complexity in their treatments of gas- and aerosol-phase chemistry, phase transfer and reactions on particle surfaces. However, this often means combining equilibrium-based treatments of aerosol processes with kinetics-based schemes, such as those for gas-phase chemical mechanisms. When multiple equilibrium-based sub-modules are used (e.g., for partitioning of inorganic and organic species), their combined use is not always straightforward. In addition, these treatments are often tightly tied to the aerosol micro-physics scheme used by the host model, and modifications to the overall mechanism, particularly for species that participate in gas and aerosol processes, is non-trivial.

We will present results from the development of a flexible treatment for chemical processes within and across gas and aerosol phases. This novel approach is designed to be accessible to both modelers and experimental chemists investigating complex chemical schemes, and permit rapid deployment to a wide range of models (e.g., box, plume, 3-D Eulerian models). This new treatment has been developed using the PartMC modeling framework and deployed in the NMMB-MONARCHv2.0 chemical weather prediction system for use at global and regional scales. Key features of the system include: 1.) simultaneous kinetics-based solving of the entire system of equations including gas- and aerosol-phase chemical reactions, emissions, deposition, photolysis, and mass-transfer; 2.) abstraction of the aerosol representation of the host model (e.g., binned, modal or particle-resolved) in which aerosols are treated as a collection of condensed phases, which can be implemented according to the scheme used by the host model without modification of the mechanism; 3.) input files in JSON format, a widely used format for structured data, that permit the entire mechanism to be described in human-readable format with elements that range in complexity from single gas-phase reactions to entire sets of UNIFAC interaction parameters; 4.) run-time processing of input files that permits changes to any part of the mechanism without recompilation of the model. Preliminary results using the modified PartMC library in the NMMB-MONARCHv2.0 model will be discussed along with its application to various host models, extension to complex gas–aerosol systems, and acceleration by GPU-based solving.