Geophysical Research Abstracts
Vol. 13, EGU2011-11583, 2011
EGU General Assembly 2011

A new method to simulate coagulation of an externally mixed particle population

Hilel Dergaoui (1), Christian Seigneur (2), Karine Sartelet (2), Edouard Debry (1), Bertrand Bessagnet (1), and Laurence Rouïl (1)

(1) Institut National de l'Environnement Industriel et des Risques (INERIS), Parc technologique ALATA BP 2, 60550 Verneuil en Halatte, France (Hilel.Dergaoui@ineris.fr), (2) Centre d'Enseignement et de Recherche en Environnement Atmosphérique (CEREA), Joint Laboratory of Ecole des Ponts ParisTech/EDF R&D, University Paris-Est, 6-8 avenue Blaise Pascal, Cité Descartes Champs-sur-Marne, 77455 Marne la Vallée Cedex 2, France

The usual way to follow the particle distribution in atmosphere is to assume particles to be internally mixed. This means that particles with same size have also the same composition, hence the same physical and chemical properties. This assumption has already been lifted in order to correctly account for the elemental carbon effect on aerosol climate forcing [Jacobson 2001] and also to study pollution near emission sources [Kleeman et al. 1997], where newly emitted particles may be present with aged transported particles, with the same size but different composition.
The representation of an externally mixed particle population in a 3D eulerian chemical transport model has already been developed [Jacobson 2002]. A sectional approach is used for particle size, whereas the mixing state is approached by introducing several particle distributions, each one being associated with one particular source or kind of composition. In addition, some mixing thresholds between distributions allow for a more accurate representation [Bowman et al. 2010].
In this communication, we present a new method to simulate coagulation and of an externally mixed particle population. Instead of introducing several distributions, the sectional approach is extended to the particle composition. That is to say the chemical composition of particles in each size section is discretized according to the percentage of one or more of its components. The entire chemical composition space can then be partitioned for each particle size.
This method allows for a rigorous treatment of coagulation, which tends to mix particles among themselves. As an example, the implementation of coagulation results in the computation of coefficients to distribute mass among size and composition sections. The advantage of this approach is first, the possibility to set composition sections as wanted and second, to choose optimally between accurate mixing state representation and cpu cost.
The principles of this method are discussed and the ability of this method to represent the aerosol mixing state is demonstrated with a 0D simulation. Future work will adress the condensation/evaporation growth with this computational formulation.

[Kleeman et al. 1997] Modeling the airborne particle complex as a source-oriented external mixture. Kleeman, M.J. and Cass, G.R. Journal of Geophysical Research. 1997. Volume 102. Pages 21355-21372.
[Jacobson 2001] Strong radiative heating due to the mixing state of black carbon in atmospheric aerosols. Jacobson, M.Z. Nature. 2001. Volume 409. Pages 695-697.
[Jacobson 2002] Analysis orf aerosol interactions with numerical techniques for solving coagulation, nucleation, condensation, dissolution, and reversible chemistry among mutliple size distribution. Jacobson, M.Z. 2002. Journal of Geophysical Research. Volume 107. D19.
[Bowman et al. 2010] A detailed aerosol mixing state model for investigating interactions between mixing state, semivolatile partitioning, and coagulation. Lu, J. and Bowman, F.M. 2010. Atmospheric Chemistry and Physics. Volume 10. Pages 4033-4046.