A study of combustion aerosols in Japan using a nonhydrostatic icosahedral atmospheric model

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An aerosol-coupled global cloud-resolving model, NICAM-SPRINTARS, developed by [1] based on the aerosol module of Spectral Radiation-Transport Model for Aerosol Species (SPRINTARS; [2]) and the global cloud-resolving model of Nonhydrostatic Icosahedral Atmospheric Model (NICAM; [3,4]) is capable to simulate the aerosol processes and distributions not only in the whole globe but also over specific regions using a stretched grid system developed by [5] as a 'seamless' model. In the present study, we develop the seamless aerosol-transport model with the spatial resolution of about 10 km to simulate aerosols around Japan, especially the Kanto region including Megacity Tokyo.

Although in some cities near mountains the present model does not always reproduce both the meteorological and aerosol fields mainly due to large spatial resolution, around the center of Tokyo it can sucessfully simulate meteorological and aerosol fields such as sulfate (Figure). In the presentation, we will discuss the performance of the newly developed aerosol model.

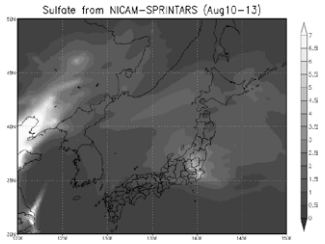

Figure 1: Simulated sulfate around Japan in unit of μg/m^3.

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Thermodynamics of solid solutions: the Margules equation and beyond

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For the thermodynamic treatment of phase equilibria the knowledge of *Gibbs free energy G* of solid solutions are essential. The thermodynamic models used for solid solutions are mostly the *regular solution*, the *Margules-*, and the *Guggenheim-equation*. The calibration of the involved parameters involves the results from phase equilibria studies. Alternatively, the lattice energy is calculated on the atomistic scale by using empirical force potentials or ab-initio calculations. Cluster expansion and applying statistical mechanics e.g. *Monte Carlo* methods are then used to evaluate *G*. For thermodynamic calculations parameterization of *the Gibbs free energy* rely then on the same models as for the thermodynamic approach.

The *regular solutions* and the *Margules equation* originate from fluid mixtures. A general approach can be applied to solids considering, that the molar mixing energy u depends on x_i and the occupancy x_j of neighboring adjacent or more distant sites. For *one* neighbor of the same site, u is:

$$u = \sum_{i=1}^{c}\sum_{j=1}^{c} x_i x_j u_{ij} \quad \text{with} \quad \Delta U_{ij} = 2u_{ij} - u_{ii} - u_{jj}$$

which gives us the *regular solution*:

$$u = \sum_{i=1}^{c} x_i u_{ii} + \frac{1}{2}\sum_{i=1}^{c}\sum_{j=1}^{c} x_i x_j \Delta U_{ij}$$

If the energy depends on *two* neighboring sites

$$u = \sum_{i=1}^{c}\sum_{j=1}^{c}\sum_{k=1}^{c} x_i x_j x_k u_{ijk} \quad \text{with} \quad \Delta U_{ijk} = 3u_{ijk} - u_{iii} - u_{jjj} - u_{kkk}$$

results in the *Margules equation* including a ternary term:

$$u = \sum_{i=1}^{c} x_i u_{iii} + \sum_{i=1}^{c}\sum_{j=i+1}^{c} x_i x_j \left(x_i \Delta U_{ij} + x_j \Delta U_{ijj}\right) + 2\sum_{i=1}^{c}\sum_{j=i+1}^{c}\sum_{k=j+1}^{c} x_i x_j x_k \Delta U_{ijk}$$

The above equation can also be written in the form:

$$u = \sum_{i=1}^{c} x_i u_{iii} + \frac{1}{3}\sum_{i=1}^{c}\sum_{j=1}^{c}\sum_{k=1}^{c} x_i x_j x_k \Delta U_{ijk}$$

This procedure can be extended to more complex interactions. If the energy of the site depends on the occupancy of *four* of the same site and *two* of a neighboring site:

$$U = \sum_{i=1}^{c_A}\sum_{m=1}^{c_B} x_i^A x_m^B u_{(iiii)(mm)} + \frac{1}{8}\sum_{i=1}^{c_A}\sum_{j=1}^{c_A}\sum_{k=1}^{c_A}\sum_{l=1}^{c_A}\sum_{m=1}^{c_B}\sum_{n=1}^{c_B} x_i^A x_j^A x_k^A x_l^A x_m^B x_n^B \Delta U_{(ijkl)(mn)}$$

It is important to note that these types of equations always split in a term for the *mechanical mixture* and one involving only parameters ΔU based on energy differences, which can be acquired by theoretical calculations for complex and arbitrary system.

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DOI:10.1180/minmag.2013.077.5.7