

AEROSOL AGING AND MIXING STATE FOCUS GROUP

Make everything as simple as possible, but not simpler. – Albert Einstein

Objective: This focus group proposes to study the sensitivity of aerosol physical and optical properties to the aerosol mixing state, and work to determine the extent to which models need to include all of this complexity. This focus group will bridge what is learned from properties and process-centered focus groups and the modeling community in order to improve the representation of aerosol mixing state in regional to global scale models.

Rationale: Mixing state is a measure of complexity, so the extent that physical and optical properties of aerosols are mixing-sensitive should be a good indicator of the level of model complexity one can expect will be required to represent aerosols in atmospheric models. To illustrate, assume for the sake of argument that aerosol CCN activity were dependent solely on particle size. Then there would be no need to track aerosol composition – particle size and number concentration alone would suffice as aerosol CCN properties are concerned. Another property, e.g. aerosol absorption, might, on the other hand, be highly sensitive to mixing state. Then some level of mixing would need to be tracked in order to get good representation of aerosol radiative properties and atmospheric heating rates – i.e. a greater level of model complexity is required in the second case.

Scientific Questions:

- Can ASR develop reliable, easy to use metrics that quantify the mixing states of aerosols? For example, how can the classic definitions, which are limited to the special cases of internal and external mixing, be extended to general mixing?
- To what extent are aerosol physical and optical properties dependent on mixing state and how can this dependence be best parameterized in models?
- How and to what level of detail does aerosol mixing state need to be included in models?
- How do such aerosol processes as anthropogenic/biogenic interactions, SOA formation, and aging in different environments affect mixing state?
- Over what time scales do aerosols become mixed to a degree so that the assumption of “internally mixed aerosols” is reasonable?
- What can single particle measurements tell us about aerosol mixing state?
- What can particle-resolved simulations tell us about aerosol mixing state?

Approach:

By its nature, this focus group is broad in scope. To be successful, it will require participation from both the measurements and modeling communities as well as from the likely aerosol properties and process-oriented focus groups currently being proposed.

Participation from the measurements community: Single particle measurements (e.g. single particle mass spectroscopy, SP2, electron microscopy) provide valuable and detailed information on individual particle size, internal composition, shape, morphology, surface properties, fractal dimension, etc. For example, the analysis of individual particle size and composition during CARES clearly indicates that at any given time particle compositions were complex: There were always a number of different types of particles with different compositions and size distributions present. While most of the particles consisted of sulfates mixed with organics, pure sulfate particles as well as pure organic particles were present, the latter containing different types of oxygenated organics and organic amines. Other particle types included fresh and processed soot particles, biomass burning aerosol, organic amines, sea salt – fresh and processed – and a small number of dust and other inorganic particles. Single particle measurements are not the only way to obtain aerosol mixing state information. Techniques requiring some degree of particle averaging can also be of great value (e.g. AMS, CCN spectrometers, tandem DMAs).

In addition to the field measurements, environmental chamber experiments are needed to obtain particle-resolved aerosol size, shape, morphology, composition, and mixing state data together with ensemble optical and CCN measurements that can be used to constrain, evaluate, and improve the models. The ultimate goal of such an integrated particle-resolved modeling and measurement strategy is to develop and evaluate a reliable and computationally efficient mixing-state framework that can be used in regional and global climate models. To the best of our knowledge, such experiments have never been performed before, but are needed to evaluate and verify the performance of detailed aerosol chemistry and dynamics models.

Participation from the modeling community: We envision a participation from modelers across all scales. The modeling efforts will be centered around developing metrics for the evolution of mixing state, performing model intercomparison and validation, as well as developing mixing state parameterizations.

Developing Metrics: Particle-resolved (PR) models are especially important for simulating the dynamics of mixing state at its most fundamental (and most detailed) level. Metrics for characterizing the evolution of mixing state remain to be developed and here PR-simulation and measurement will play a major role.

These metrics should be simple to use and the two communities (modeling and measurements) should strive to develop common metrics that facilitate model validation.

Model intercomparison, benchmarking, and validation: Models on the regional to global scale will of necessity continue to employ simplified aerosol representations. These models need to be optimized and validated against both measurements and PR-type simulations.

Developing mixing state parameterizations: A challenge is to develop simplified and computationally efficient models that reliably include mixing state information. For example: a model that tracks particle number and bulk composition might also include a hidden local parameter like photochemical age (ratio of gas phase NO_x to NO_y concentrations). This would allow particles of the same composition, which otherwise appear identical to the aerosol module, to be subsequently treated differently, e.g. they could be assigned different CCN potentials if the air masses they inhabit have different photochemical age. For developing such parameterizations we foresee employing modeling approaches from the process level to the global scale. Participation of the climate modeling community is especially important if the best level of reduction in model complexity is to be achieved.