Coupling the Stochastic Particle-Resolved Aerosol Model PartMC with MOSAIC and WRF-1D

Jeffrey Curtis, Nicole Riemer, Matthew West University of Illinois at Urbana-Champaign

What Are Particle-Resolved Aerosol Models?

- No bins or modes
- Particles as vectors
- Treating multidimensional size distribution



	Particle 1	Particle 2	Particle 3
BC	3	10	1
SO ₄	12	3	4
OC	5	8	2

Why Particle-Resolved Aerosol Models?

- Advantages:
 - Efficient representation of multidimensional size distribution
 - Advantageous whenever the per-particle-composition (= "mixing state") is of interest: No assumptions about mixing state are needed.
- Disadvantage: Expensive to run
 - Each particle costs the same as one section or mode.
 - Need 1,000 to 100,000 particles





particle-resolved

Box Model PartMC-MOSAIC

PartMC: Particle-resolved Monte Carlo aerosol model

- Stochastic treatments for emission, dilution, and coagulation
- Riemer, N., M. West, R.A. Zaveri, and R.C. Easter, Simulating the evolution of soot mixing state with a particle-resolved aerosol model, *JGR*., 114, D09202, 2009.

MOSAIC: Model for Simulating Aerosol Interactions & Chemistry

- Deterministic treatments for gas photochemistry, aerosol thermodynamics, and dynamic gas-particle mass transfer
- Zaveri, R.A., R.C. Easter, J.D. Fast, and L.K. Peters, Model for Simulating Aerosol Interactions and Chemistry (MOSAIC), JGR., 113, D13204, 2008.

Aerosol Properties Modules:

- Kappa-Köhler Model for CCN: Petters, M.D. and S.M. Kreidenweis, A single parameter representation of hygroscopic growth and cloud condensation nucleus activity, *Atmos. Chem. Phys.*, 7, 1961-1971, 2007.
- ACKMIE Shell-Core Model for Optics: Ackerman, T.P. and O.B. Toon, Absorption of visible radiation in atmospheres containing mixtures of absorbing and non-absorbing particles, *Appl. Optics*, 20, 3661-3668, 1981.

Evolution of Black Carbon Mixing State



Application 1: Benchmarking McGraw, Leng, Zhu, Riemer, West, J. Phys.: Conf. Series, 125, 2008



Figure 2. Evolution of total particle number (upper left panel) showing exact QMOM (curve) and particle-resolved simulation (markers) results. Remaining panels show particle number fraction for each population: long-dashed curves, QMOM with 7-moment tracking; short dashed curves, QMOM with 14-moment tracking; markers, particle resolved simulation.

Application 2: Assessing the Importance of Mixing State

Zaveri, Barnard, Easter, Riemer, West, JGR, 115, D17210, 2010



Application 3: Quantifying Black Carbon Aging Timescales (Riemer, West, Zaveri, Easter, J. Aerosol Sci., 41, 143-158, 2010)



Connecting PartMC-MOSAIC with Laboratory Measurements

New project funded by ASR: Collaboration of Tami Bond, Mark Rood, Nicole Riemer

Isolating Weakly and Strongly-Absorbing Classes of Carbonaceous Aerosol: Optical Properties, Abundance and Wet Removal



Adding Transport: Coupling PartMC-MOSAIC with WRF Single Column Model



- Stochastic aerosol transport: Diffusion coefficient is reinterpreted as probability for moving grid cells.
- Parallelization and superparticles enable fast simulation.
- More on the numerical method and model verification: See poster by Jeff Curtis today

24-h Urban Plume Simulation

Summary and Outlook

- Particle-resolved model PartMC-MOSAIC as a way to model multidimensional aerosol size distributions without a priori assumptions about mixing state.
- Going beyond the box: Current efforts focus on coupling PartMC-MOSAIC to a 1D version of WRF.
- Next steps: Investigate interaction of transport and aerosol microphysics and chemistry
 - Aerosol aging, spatially resolved
 - Quantifying mixing state effects on aerosol radiative impacts
 - Connecting to field measurements
 - Extension to 3D