Proposed Modeling Improvements and Implementation Relevant to the Focus Questions

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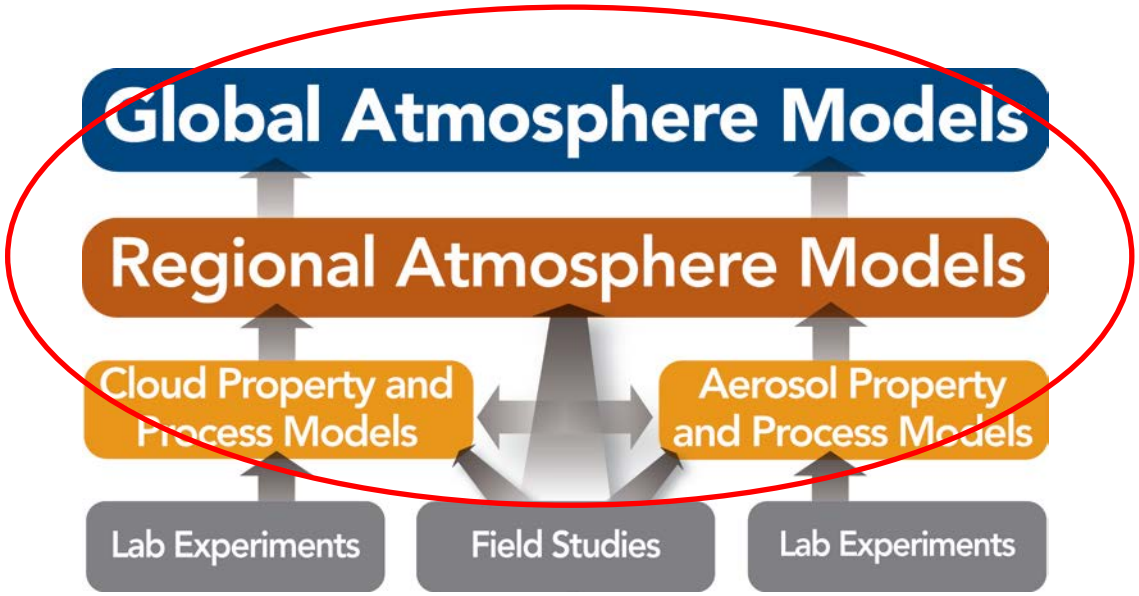
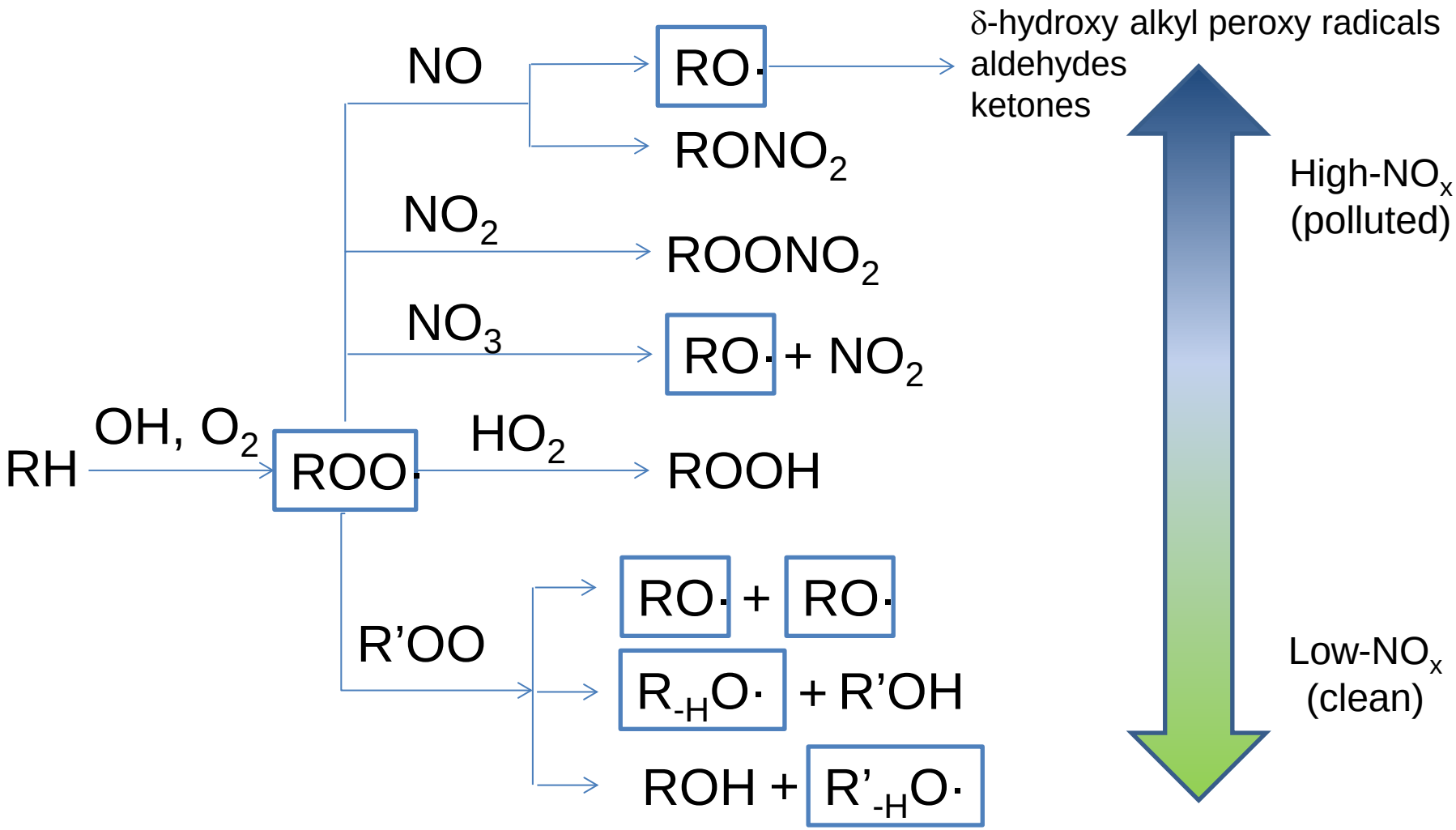
A-B Interactions Focus Group strategy



- Focus on:
  - Fate of ROO radicals in the gas phase
  - SOA physical state and morphology
  - Particle phase reactions

Focus Area 1: Fate of ROO Radicals in the Gas Phase



Focus Area 1: Fate of ROO Radicals in the Gas Phase Modeling Approach

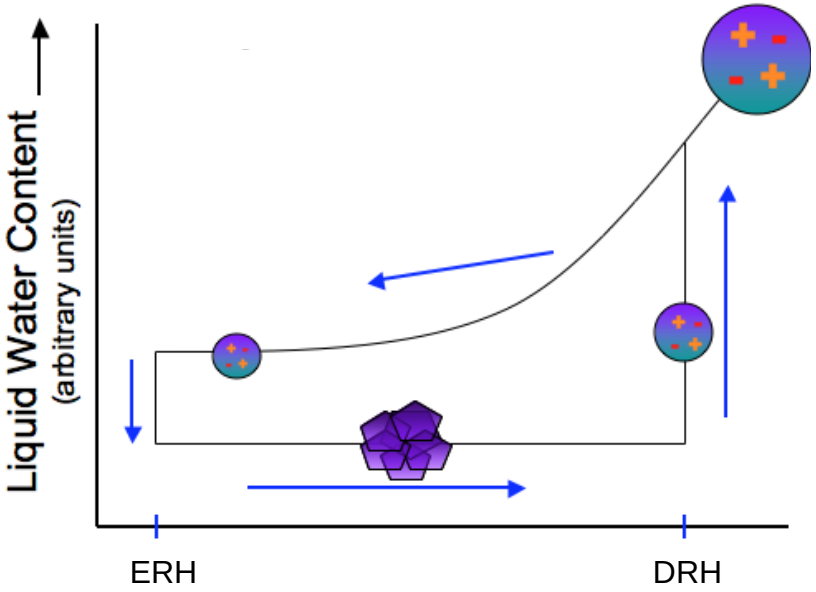
Laboratory & Field Measurements of key gas-phase species and size-distributed aerosol composition under varying AVOC+BVOC/NO_x

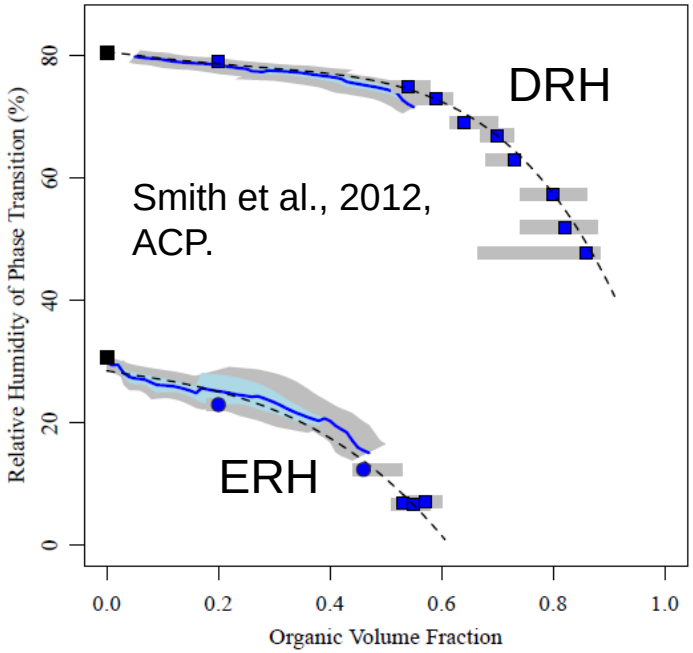
Detailed gas-phase mechanism such as MCM, GECKO to provide insights into the fate of ROO radicals under polluted and clean conditions

Condensed gas-phase mechanism + gas-particle partitioning treatment that predicts size-distributed organic-inorganic aerosol composition

Focus Area 2: SOA Physical State and Morphology

- Phase state of mixed organic-inorganic aerosols (liquid, semi-solid, solid, phase separation, deliquescence, efflorescence, water uptake)
- Physical properties as a function of composition (bulk diffusivity, surface tension)

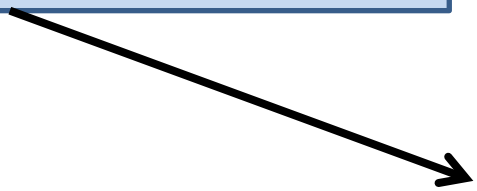




Focus Area 2: SOA Physical State and Morphology Modeling Approach

Laboratory and Field Measurements of phase-state, morphology, and phase transition behavior of mixed organic-inorganic aerosols

Detailed thermodynamics models such as E-AIM, AIOMFAC to provide benchmark calculations

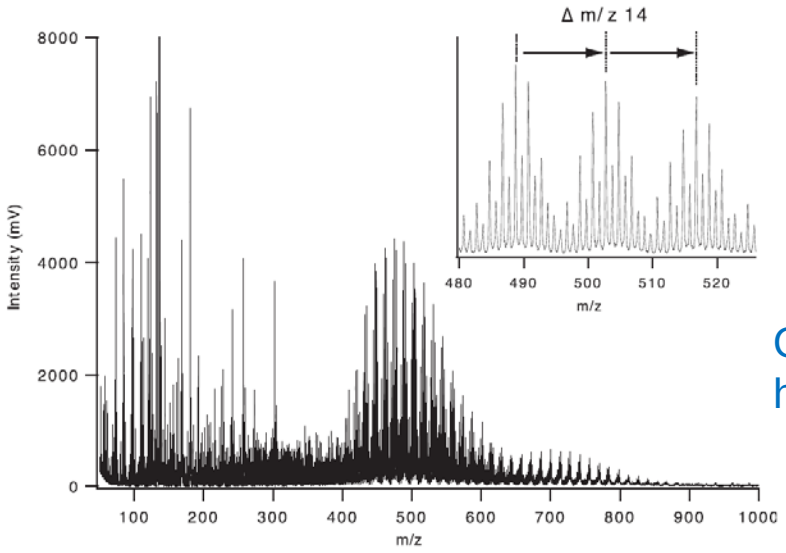


Parameterized treatment as function of O:C ratio, functional groups, etc.

Focus Area 3: Particle Phase Reactions

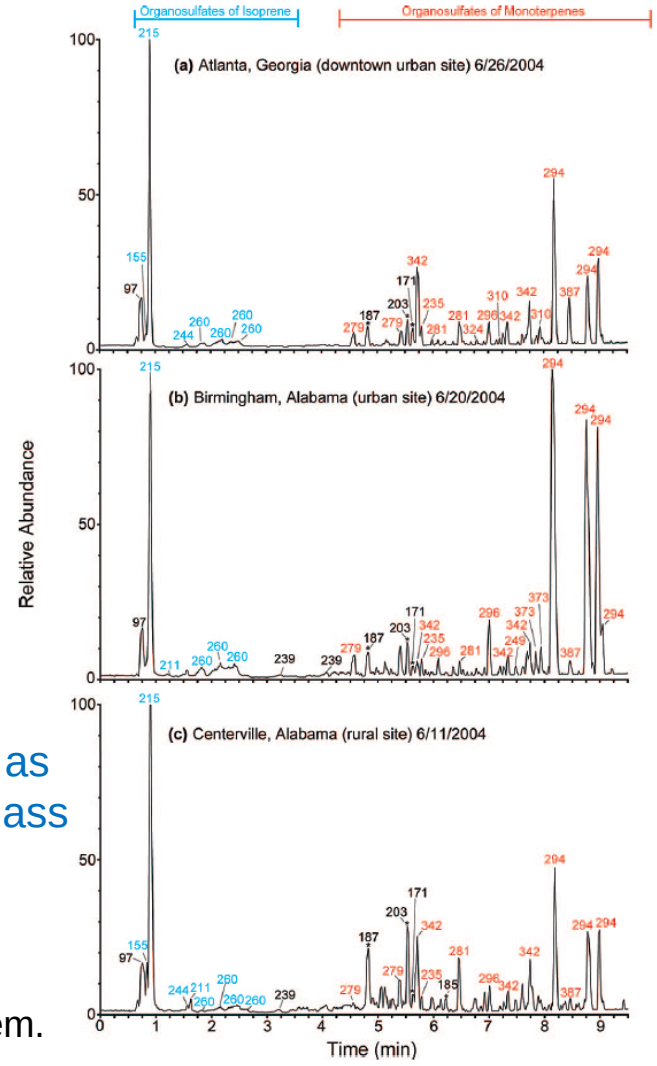
- Particle-phase reactions can lead to formation of non-volatile species such as oligomers, organosulfates, etc. in the presence of acidic sulfate particles.
- Increase particle viscosity (semi-solid), slow down mass transfer kinetics, form brown carbon, affect CCN activity.

Oligomer fraction as high as 50% of SOA mass



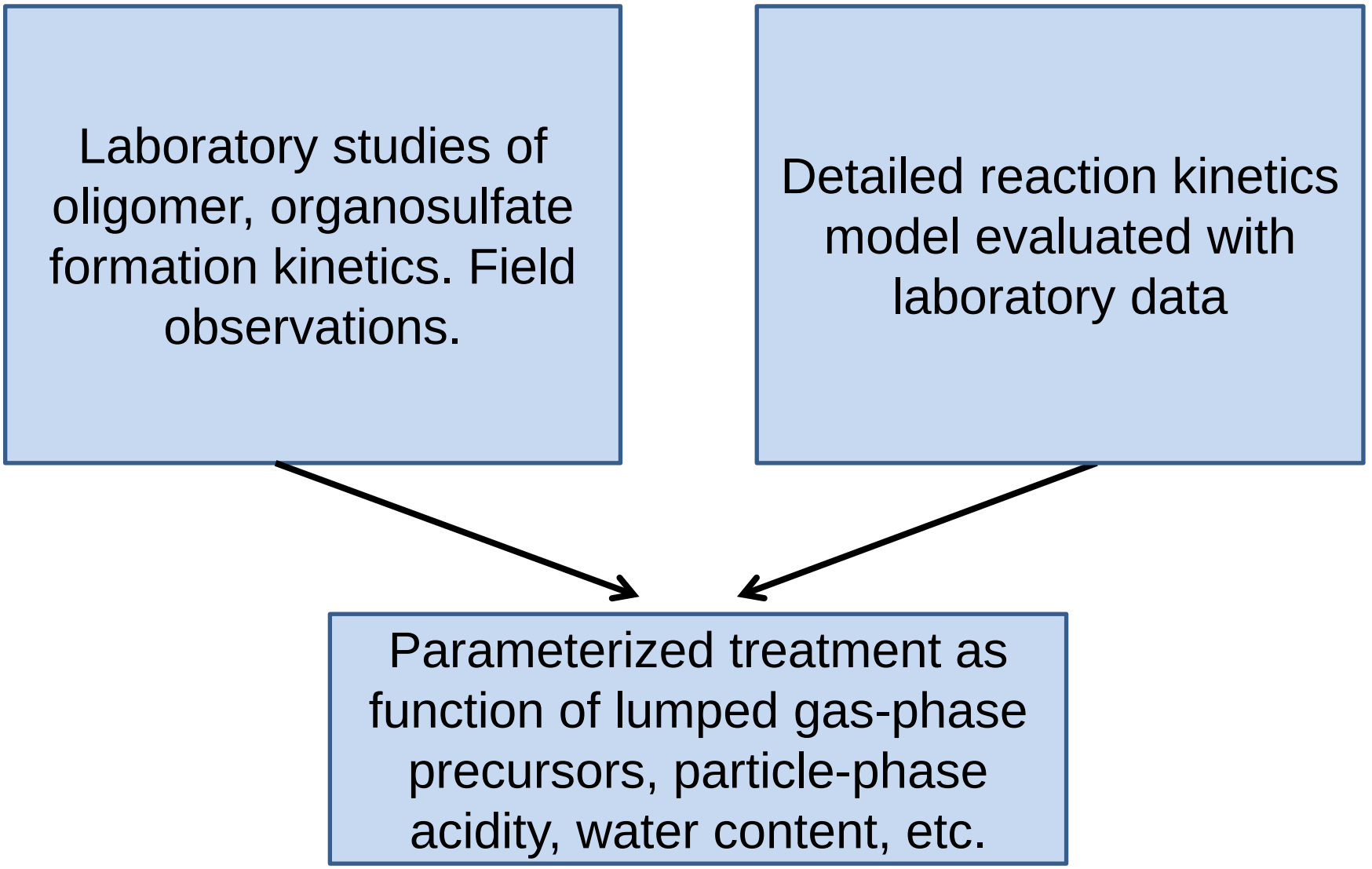
Kalberer et al., 2004, Science

Organosulfate fraction as high as 30% of SOA mass

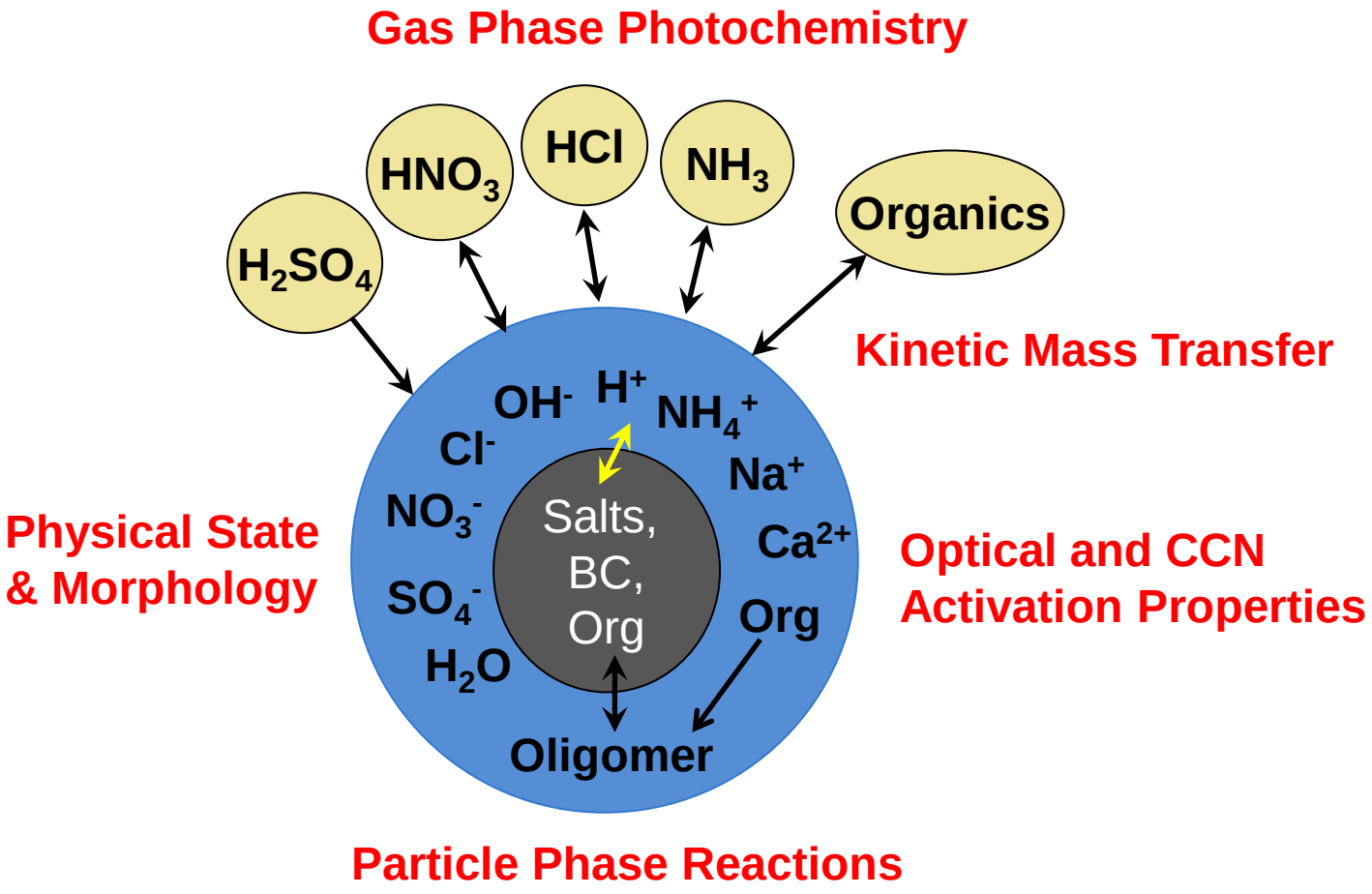


Surratt et al., 2008, J. Phys. Chem.

Focus Area 3: Particle Phase Reactions Modeling Approach



Envisioned Unified Aerosol Model

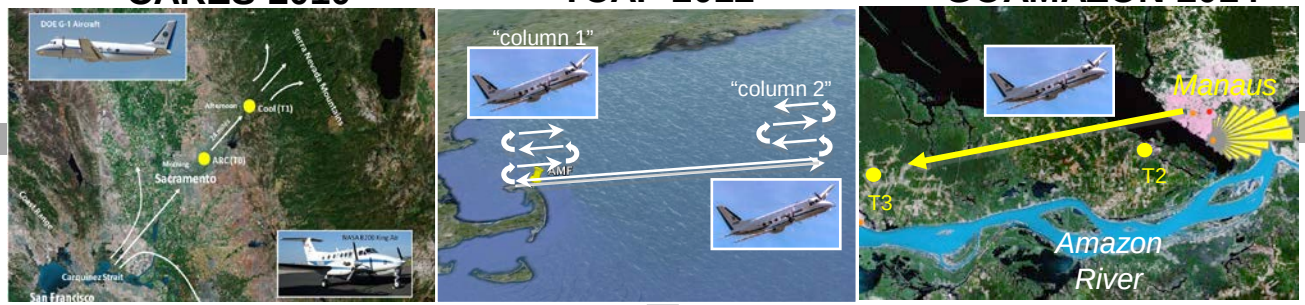


Measurements-to-Models Example

CARES 2010

TCAP 2012

GOAMAZON 2014



Use field data to guide controlled experiments

Use field data to evaluate regional model

Use lab and field data for local closures and constrained model evaluations

Field measurements

Online Chamber Experiments

Offline Physical and Chemical Analyses

Laboratory measurements

MOSAIC & PartMC-MOSAIC

Aerosol Property & Process Models

WRF-MOSAIC

Regional Model

Aerosol Modeling Testbed

CAM5-MOSAIC

Global Model

Improve and validate specific aerosol property & process model treatments

- gas-phase chemistry • new particle formation
- mass transfer kinetics • phase state thermodynamics
- particle-phase reactions • mixing state
- optical properties • CCN activation

Evaluate global climate impacts of improved model treatments

Summary

- Develop and evaluate efficient SOA model to investigate impacts of A-B interactions at regional and global scales, with a focus on:
  - Fate of gas-phase ROO radicals (NO_x dependence)
  - SOA physical state (organic-inorganic interactions)
  - Particle phase reactions (oligomer, organosulfate, etc.)

- Foster collaborative and integrated efforts for laboratory, field, and modeling studies with ASR.