Modal and Sectional Aerosol Modules

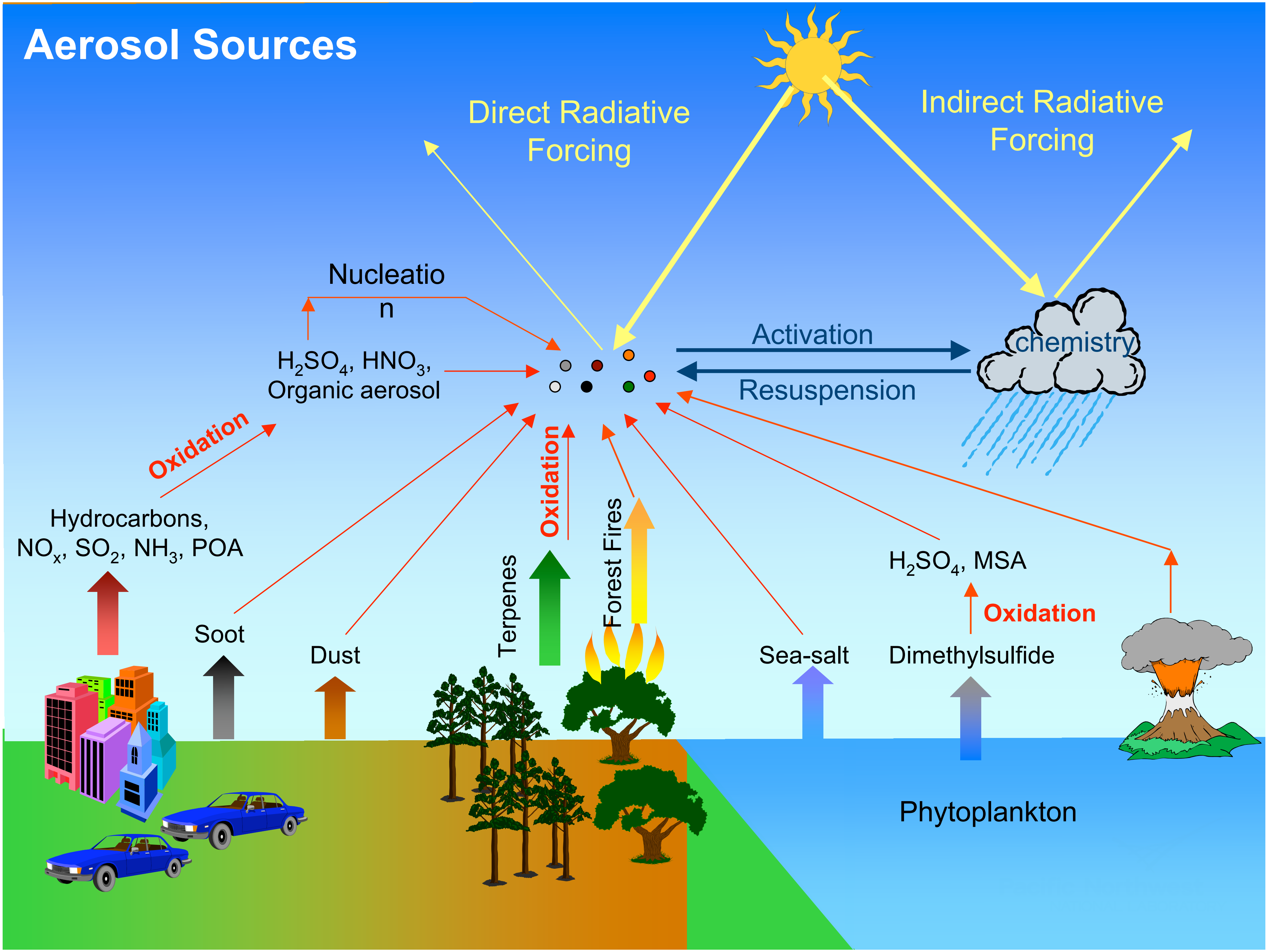
Rahul Zaveri
Pacific Northwest National Laboratory

2008 WRF-chem Tutorial
July 23, Boulder, CO

rahul.zaveri@pnl.gov

Overview

- Background
- Modal and Sectional Aerosol Modules in WRF-Chem
- Aerosol Thermodynamics and Gas-Particle Partitioning
- Some Results on Module Evaluation
- Future Updates
- Closing Remarks


Aerosol Sources
Direct Radiative Forcing
Indirect Radiative Forcing
Nucleation
H_2SO_4, HNO_3, Organic aerosol
Activation
chemistry
Resuspension
Oxidation
Hydrocarbons, NO_x, SO_2, NH_3, POA
Soot
Dust
Terpenes
Oxidation
Forest Fires
Sea-salt
H_2SO_4, MSA
Oxidation
Dimethylsulfide
Phytoplankton

Background

- **Atmospheric particles sizes span three orders of magnitude**
  - Ranges from a few nanometers to a few micrometers
- **They can be composed of a wide variety of compounds**
  - SO4, CH3SO3, NO3, Cl, CO3, NH4, Na, Ca, K, Mg, other minerals and metal oxides, black carbon, primary organic mass, secondary organic mass, water, etc.
  - Not all particles contain all the above species – they are externally mixed depending on their source/formation and processing history.
  - Different species and their mixtures have different properties
- **A number of processes affect their size, number and mass concentrations, composition, and physico-chemical properties.**
  - Gas and heterogeneous chemistries, gas-particle partitioning, coagulation, cloud and ice nucleation (*shifts mass from one form/phase to another*)
  - Dry and wet deposition (*removes it completely*)

Background

- **Urban to global scale modeling of aerosol size, number, mass, composition, and their properties is not an easy task!**
- **Scientifically challenging**
  - Many processes are still poorly understood at a fundamental level
  - Significant gaps in data still exist
- **Computationally difficult**
  - Numerical models of the various aerosol processes need to be computationally efficient and accurate
  - Require as little memory as possible

WRF-chem Aerosol Modules (official release)

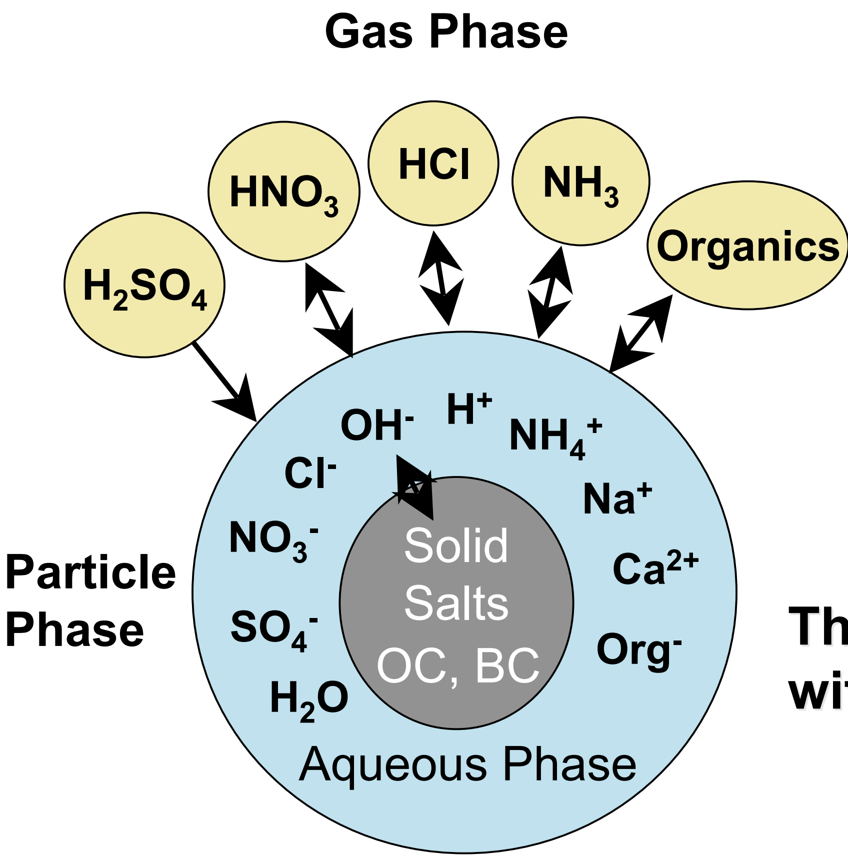
- **GOCART**
  - Bulk aerosols (simple chemistry)
  - **Chin, M., et al. (2000) Atmospheric sulfur cycle simulated in the global model GOCART: Model description and global properties. JGR., 105, 24,671-24,687.**
- **MADE-SORGAM**
  - Modal size distribution
  - **Ackermann I.J. et al. (1998) Modal Aerosol Dynamics Model for Europe: Development and first applications. Atmos. Environ., 32(17), 2981-2999.**
  - **Schell B. et al. (2001) Modeling the formation of secondary organic aerosol within a comprehensive air quality model system. JGR, 106(D22), 28,275-28,293.**
- **MOSAIC**
  - Sectional size distribution
  - **Zaveri R.A. et al. (2008) Model for Simulating Aerosol Interactions and Chemistry (MOSAIC). JGR, 113, D13204, doi:10.1029/2007JD008782.**

Aerosol Size Distribution

Sub-Module Comparison

Process	MADE-SORGAM	MOSAIC
Homogeneous nucleation (new particle formation)	**$H_2SO_4 + H_2O$** Wexler et al. [1994]	**$H_2SO_4 + H_2O$** Wexler et al. [1994]
Coagulation	**Brownian Kernel** Whitby et al. [1991]	**Brownian Kernel** Jacobson et al. [1994]
Thermodynamics (inorganic activity coefficients)	**Bromley** Bromley [1973]	**MTEM** Zaveri et al. [2005a]
Thermodynamics (equilibrium phase state)	**ISORROPIA** Nenes et al. [1998]	**MESA** Zaveri et al. [2005b]
Gas-particle partitioning (condensation + reversible)	**Dynamic** Ackermann et al. [1995]	**Dynamic** Zaveri et al. [2008]

Thermodynamics & Gas-Particle Partitioning



Dynamic and reversible mass transfer between the gas and particle phases

Thermodynamic equilibrium within the particle phase

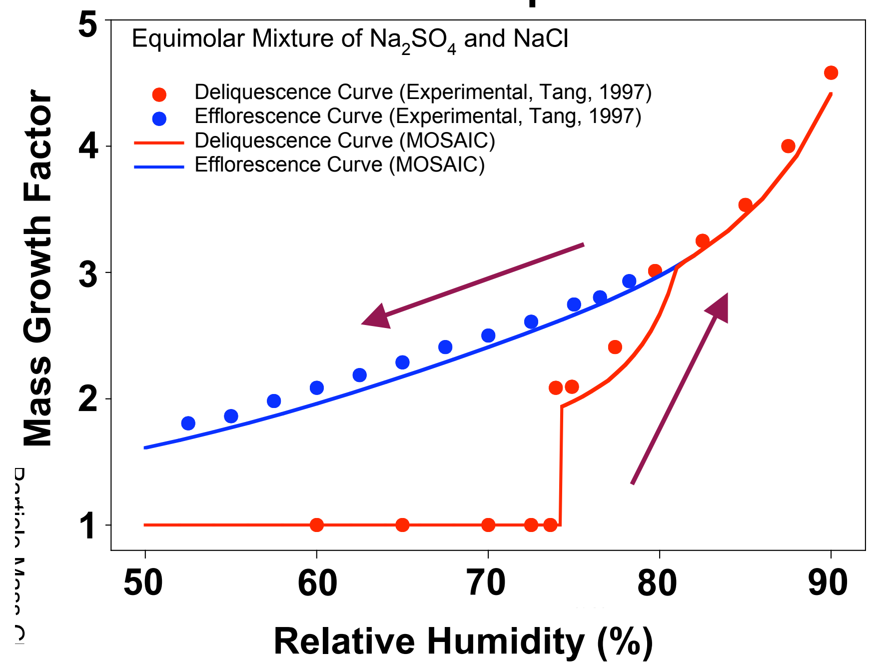
- **Together these processes typically represent the most numerically difficult and expensive portion of the overall aerosol module!**

Pacific Northwest NATIONAL LABORATORY

Aerosol Thermodynamics

- **Mutual deliquescence point**
- **Solid-liquid equilibrium**
- **Equilibrium water content**
- **Water hysteresis**

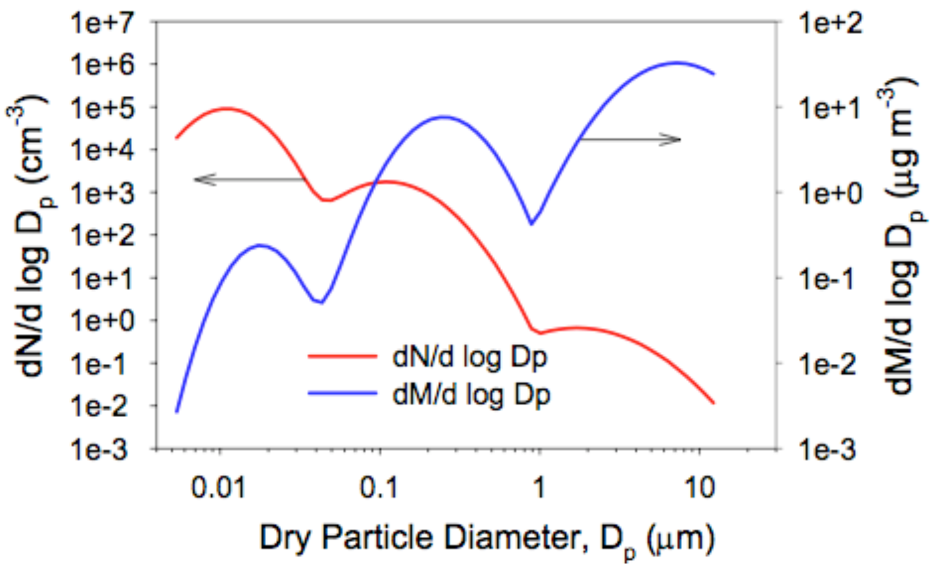
Sea-salt deliquescence



A good treatment for thermodynamics is needed for moderate to low RH values since it determines the particle size and composition, which have a profound effect on the aerosol optical properties

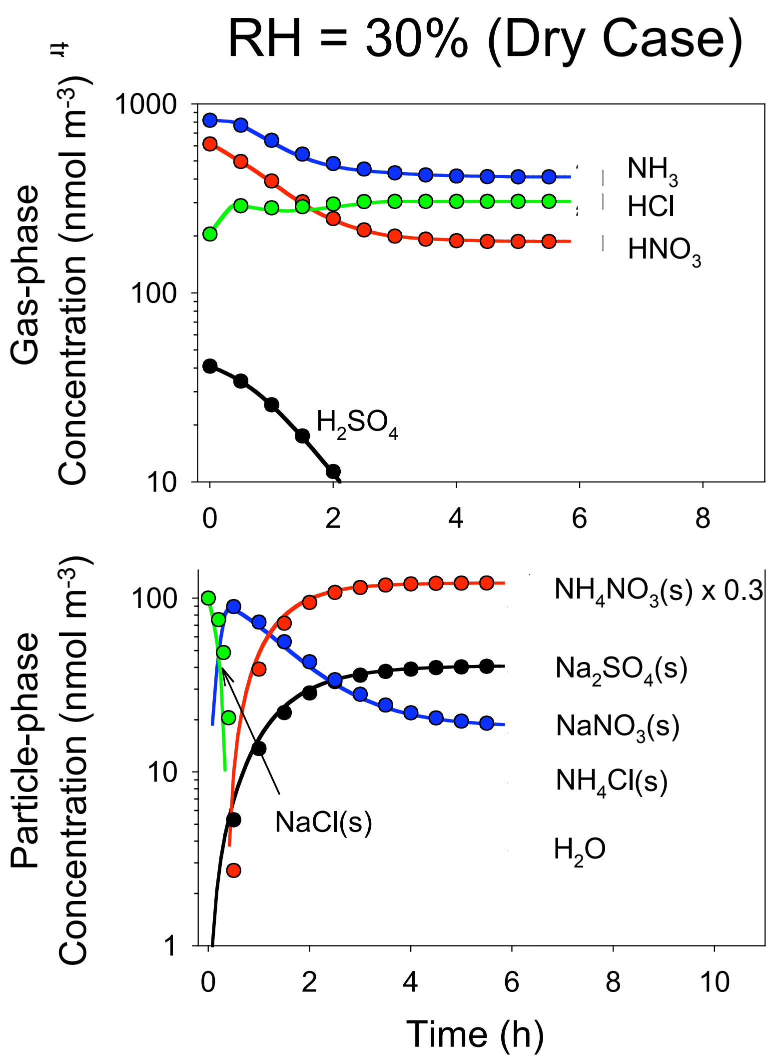
Gas-Particle Partitioning

- Mass transfer time scales range from a few seconds for small particles to a few hours for large particles
- The coupled gas-particle mass transfer ODEs are extremely stiff
- Conventional ODE solvers are very slow and/or lead to oscillatory solutions (e.g., due to numerical fluctuations in pH)



An efficient and accurate solver is needed for gas-particle mass transfer ODEs since they determine the particle size and composition evolution as a function of time.

Evaluation of Modules

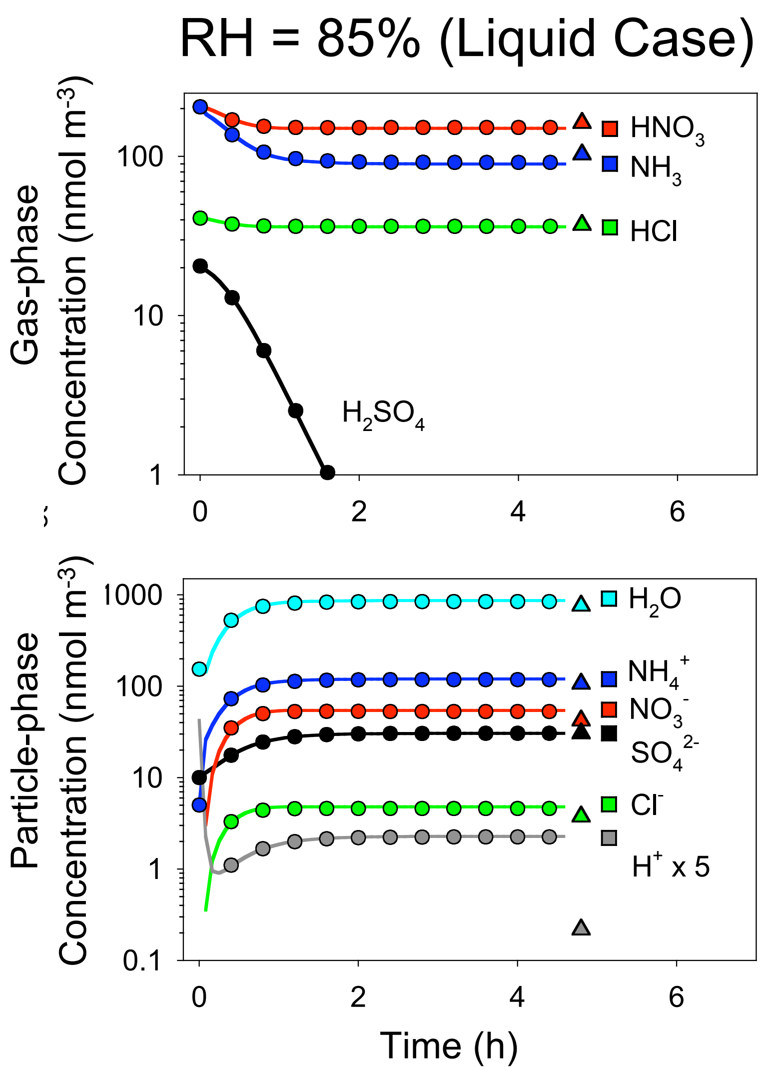


LSODES = benchmark for solving gas-particle mass transfer ODEs

MOSAIC = dynamic mass transfer coupled with thermodynamics

Pacific Northwest NATIONAL LABORATORY

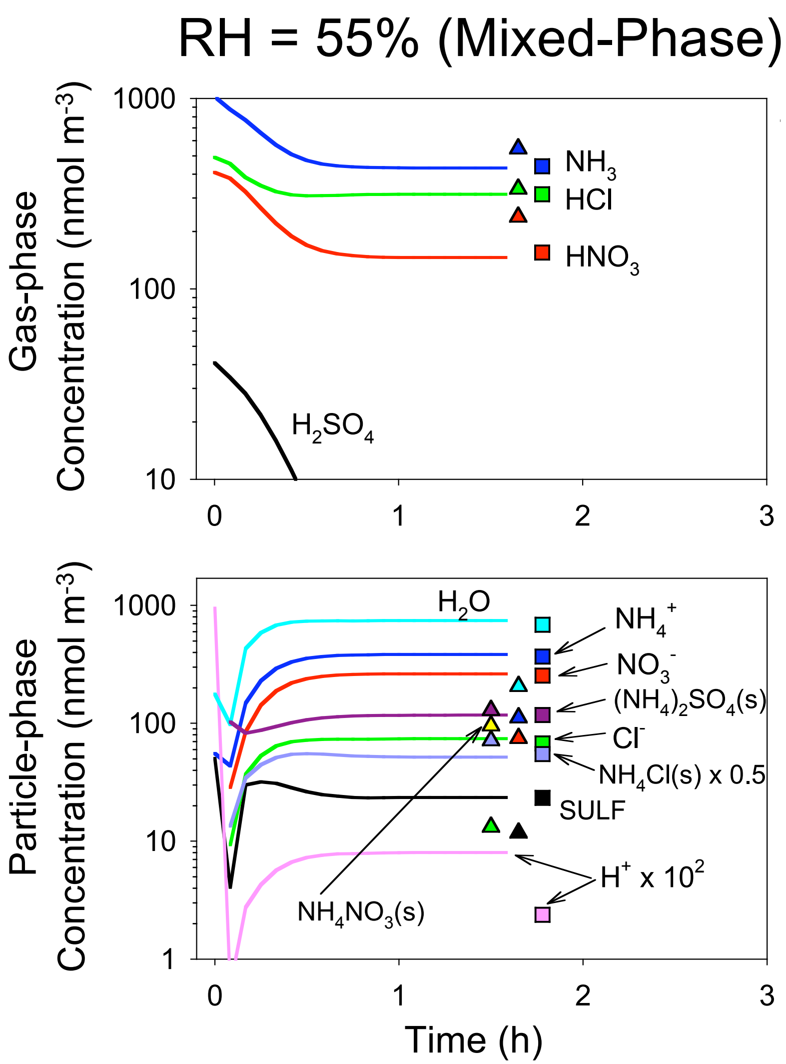
Evaluation of Modules



- LSODES = benchmark for solving gas-particle mass transfer ODEs
- AIM = benchmark for equilibrium thermodynamics
- ISORROPIA = thermodynamics module used in MADE-SORGAM
- MOSAIC = dynamic mass transfer coupled with thermodynamics

Pacific Northwest NATIONAL LABORATORY

Evaluation of Modules



LSODES = benchmark for solving gas-particle mass transfer ODEs

AIM = benchmark for equilibrium thermodynamics

ISORROPIA = thermodynamics module used in MADE-SORGAM

MOSAIC = dynamic mass transfer coupled with thermodynamics

Pacific Northwest NATIONAL LABORATORY

Comparison of CPU Times

Test Case	MOSAIC, Average CPU time (μs) per bin per 5 min Integration Interval	ISORROPIA, CPU time (μs) per Equilibrium Calculation
Case 1	13	3.5
Case 2	20	418
Case 4	32	18
Case 5	37	52
Case 6	41	44
Case 7	40	65
Case 8	190	390
Case 9	266	107
Case 11	15	246
Case 12	32	43
Case 13	25	593
Case 14	14	46

Comparison of CPU Times

SCAQS 1987 Case: 3-day simulation

Module/Model	Process	Avg. CPU Time (ms) per Grid Cell per Hour	Relative CPU time (%)
Augmented CBM-Z	Gas photochemistry	2.5	12.5
MOSAIC (8 bins)	Dynamic aerosol chemistry and microphysics	12	60
Mie & Fast-J	Aerosol optics, radiative transfer, and photolysis rates	2.5	12.5
Modified Bott's Scheme	Horizontal and vertical transport	1.8	9
Miscellaneous	Input/output and other miscellaneous calculations	1.2	6
3-D PEGASUS (offline model)	**Total**	**20**	**100**

CPU times on a 3.0 GHz Intel Xeon

Future Updates

- **Secondary organic aerosol (SOA)**
  - Current schemes/modules severely underpredict SOA mass compared to observations
  - Newer (and hopefully better!) SOA modules are being developed and will be added in the future
- **Externally-mixed aerosol representation**
  - Current aerosol modules assume internally mixed modes and bins
  - Mixing-state will be resolved in the future updates to MOSAIC

Closing Remarks

- **All models are wrong! Some are useful (if applied appropriately)**
- **Get to know your aerosol modules better**
  - All modules are not created equal
  - Learn about their strengths and limitations (read papers!)
- **Check with developer if you are trying something new**
  - Most aerosol modules are not plug-n-play
  - Adding new chemistry and processes to existing aerosol modules requires caution

Acknowledgements

- Dr. Anthony Wexler and Dr. Simon Clegg for their web-based AIM thermodynamics models.

- Dr. Athanasios Nenes, Georgia Tech, for his efforts in the intercomparison of MOSAIC and ISORROPIA.

- DOE's Atmospheric Science Program and NASA Earth Science Enterprise for funding the development and evaluation of MOSAIC.