Implementation of CBM-Z, MOSAIC, and Aerosol-Radiation-Cloud-Chemistry Interactions in WRF-chem

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Aerosol Climate Initiative

A General Description

An Overview of the Processes and Capabilites Associated with CBM-Z, MOSAIC, and Aerosol-Radiation-Cloud-Chemistry

Background

Explanation for Coding Style in WRF-chem

First A Brief History …

- CBM-Z, Fast-J, and an early version of MOSAIC in WRF-chem originated from the PEGASUS off-line chemical transport model
- Then, aerosol-radiation-cloud-chemistry interactions were added
- We are currently adding more capabilities, making modules more generic, and trying to follow WRF coding guidelines
- Our overall motivation is to use the model to better understand the local to regional-scale evolution of particulates and their effect on radiation, clouds, and chemistry

For more information and updates:

- PNNL atmospheric sciences: www.pnl.gov/atmospheric/index.stm
- PNNL modules: www.pnl.gov/atmospheric/research/wrf-chem, including capabilities, current research, and publications

Trace Gas Chemistry

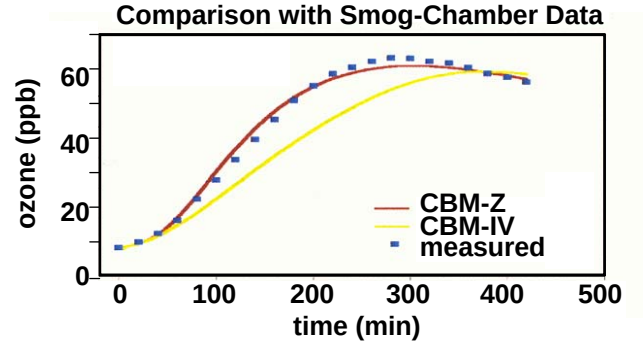
CBM-Z Mechanism for NOx-VOCs-oxidants

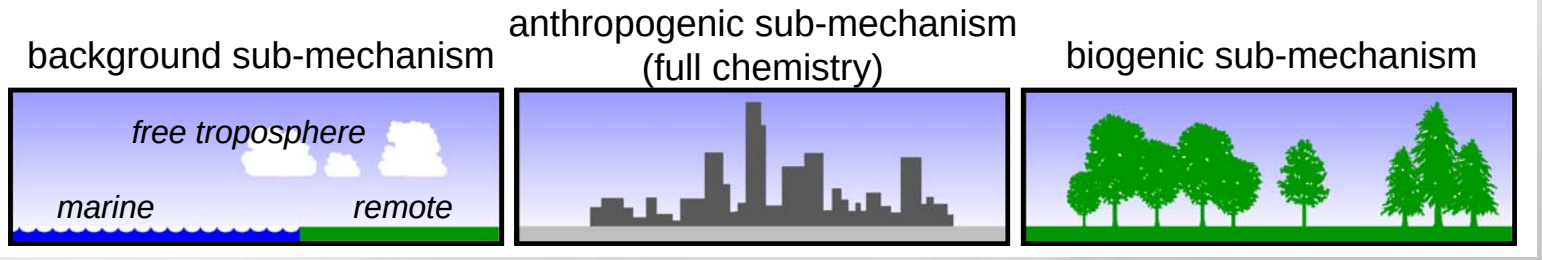
- CBM-Z extends the CBM-IV to include reactive long-lived species and their intermediates, isoprene chemistry, optional DMS chemistry, etc.
- Lumped-structure approach for organic species and reactions
- 55 prognostic species and 134 reactions
- Numerical integration uses RODAS ODE solver
- Regime-dependent sub-mechanisms to reduce computational time
- Dry-deposition velocities: series-resistance approach [*Wesley*, 1989]

<u>organic species</u>

RADM: based on similar molecular structure

CBM-Z: based on similar carbon bonds

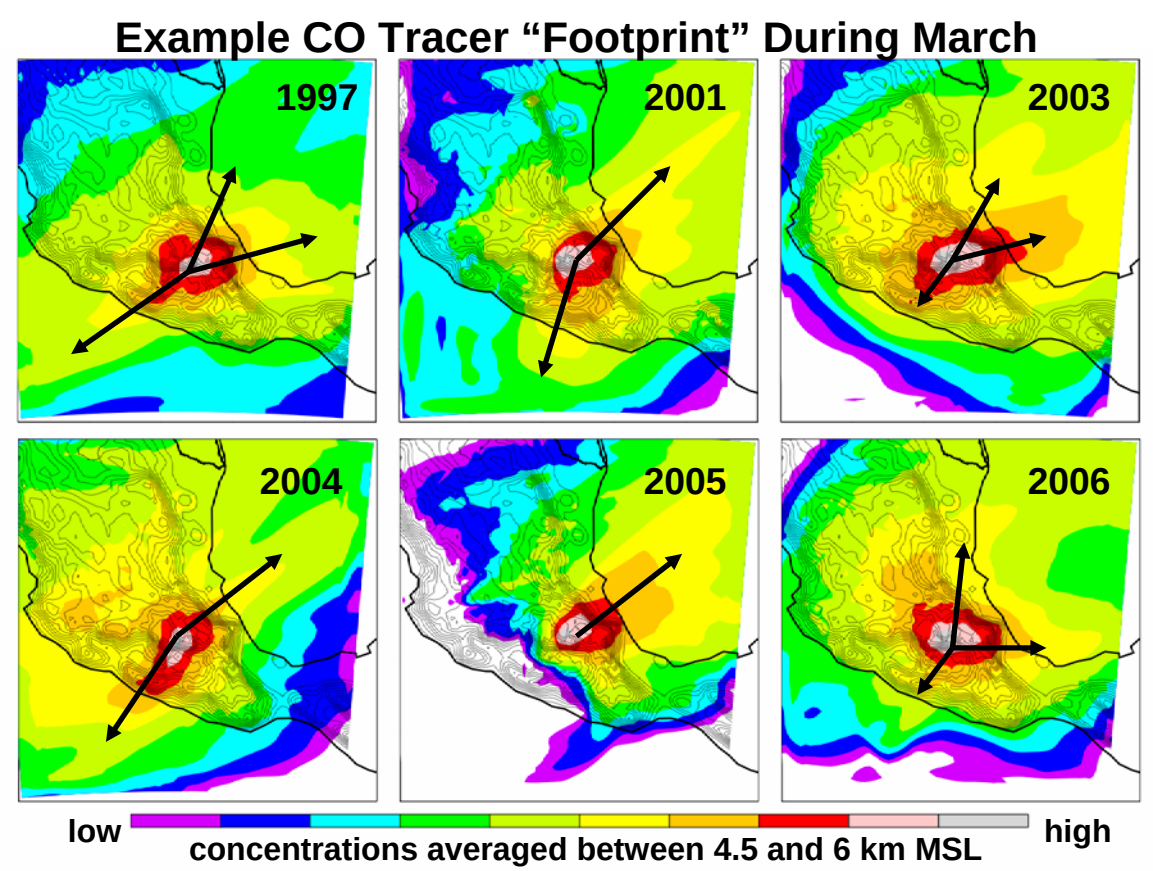




Tracer Option

Package for Transport and Mixing of Passive Scalars

- Emission, transport, vertical mixing, deposition only for chem_opt = 13
- Up to 6 tracers, hijack CO, NO, SO2, ALD, HCHO, ORA2 arrays
- Need to modify initial and boundary conditions for desired application



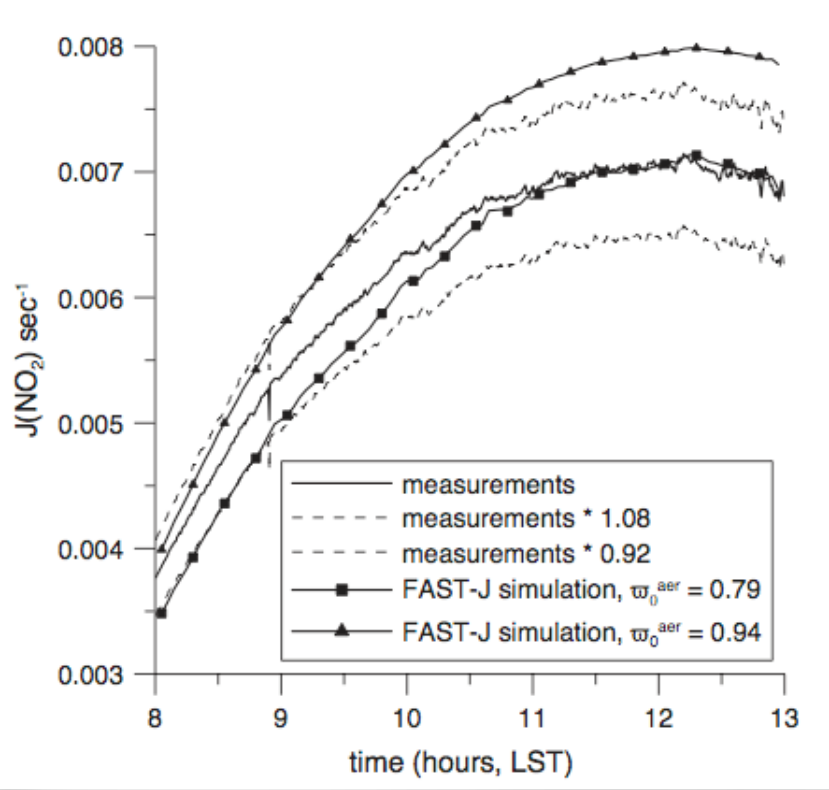
Computationally efficient - multi-month simulations feasible

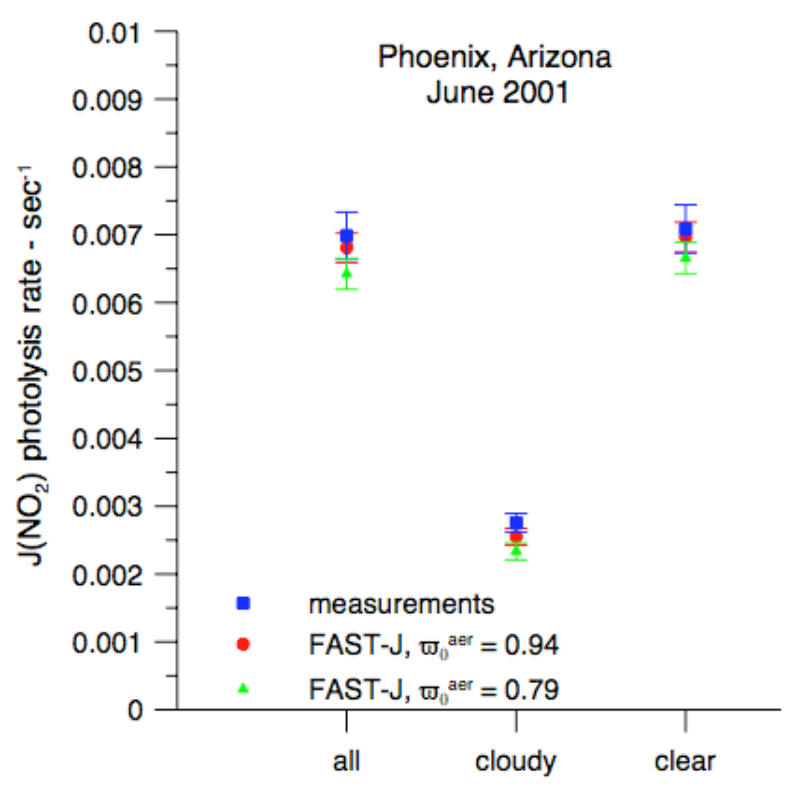
Used model to show that transport pathways during 2006 MILAGRO field campaign were similar to other years

Photolysis

Fast-J Scheme for Photolysis Rates for Gas-Phase Photochemistry

- Photolysis rates for 23 reactions based on [*Wild et al*., 2000] depend on predicted vertical profiles of ozone, aerosols, and clouds
- CBM-Z works with either FAST-J or TUV
- FAST-J and TUV have not yet been directly compared

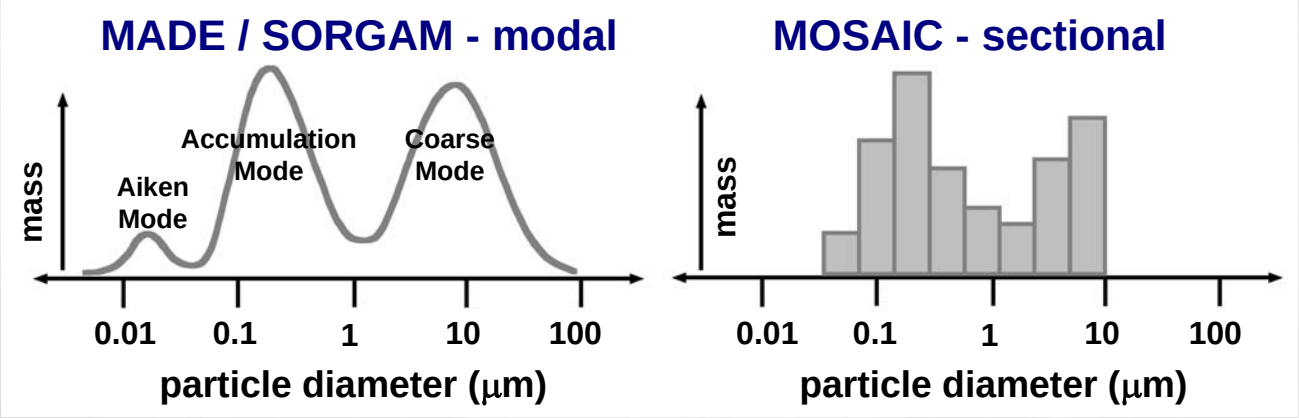




Aerosol Chemistry (1)

Model for Simulating Aerosol Interactions and Chemistry (MOSAIC)

- Sectional size representation (4 or 8 bins), 8 bin option requires 112 prognostic species
- Transfer of mass between bins uses either a two-moment approach (default) or a moving center approach for the dynamic equations for mass and number



Species				Currently Disabled	
sulfate	SO_4	other inorganics	OIN	calcium	Ca
nitrate	NO_3	organic matter	OC	carbonate	CO_3
ammonium	NH_4	black carbon	BC	methanesulfonate	CH_3SO_3
chloride	Cl	liquid water	water	**To activate, just add to Registry**	
sodium	Na	number	num		

Aerosol Chemistry (2)

Aerosol Physics

- **Nucleation:** Binary nucleation (H_2SO_4 - H_2O) of *Wexler* [1994] (default); ternary nucleation option should not be used
- **Coagulation:** *Jacobson et al.* [1994] with a Brownian kernel
- **Dry deposition:** *Binkowski and Shankar* [1995] using wet size of particle

Nucleation and Coagulation new since version 2.1

Secondary Organic Aerosol Formation

- None at present for MOSAIC
- Rahul Zaveri has developed a box-model version of MOSAIC with SOA treated similar to SORGAM is nearly complete and is expected to be implemented in WRF-chem this year
- Other groups to implement SOA with WRF-chem ?

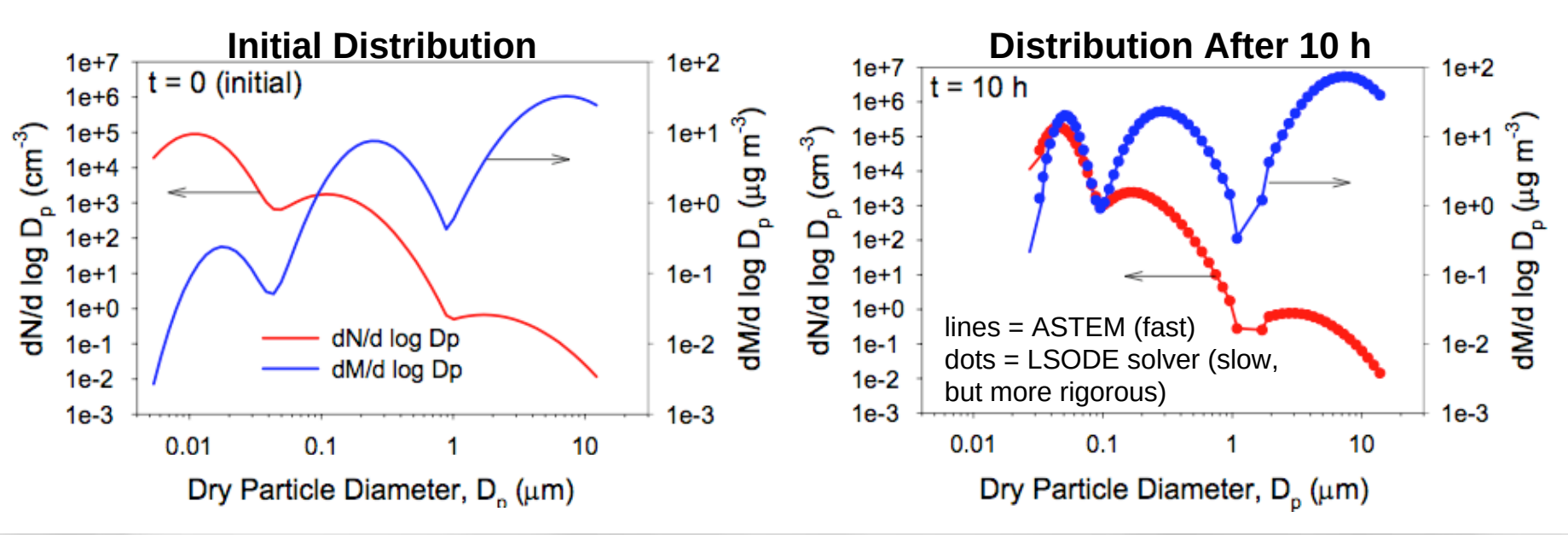
Aerosol Chemistry (3)

Thermodynamics

- **MTEM:** mixing rule for activity coefficients of various electrolytes in multi-component aqueous solutions
- **MESA:** thermodynamic equilibrium solver for solid, liquid, or mixed-phase state of aerosols
- **ASTEM:** dynamic integration of the coupled gas-aerosol partitioning differential equations

numerically efficient and accurate

[Zaveri et al. 2005ab, 2007]

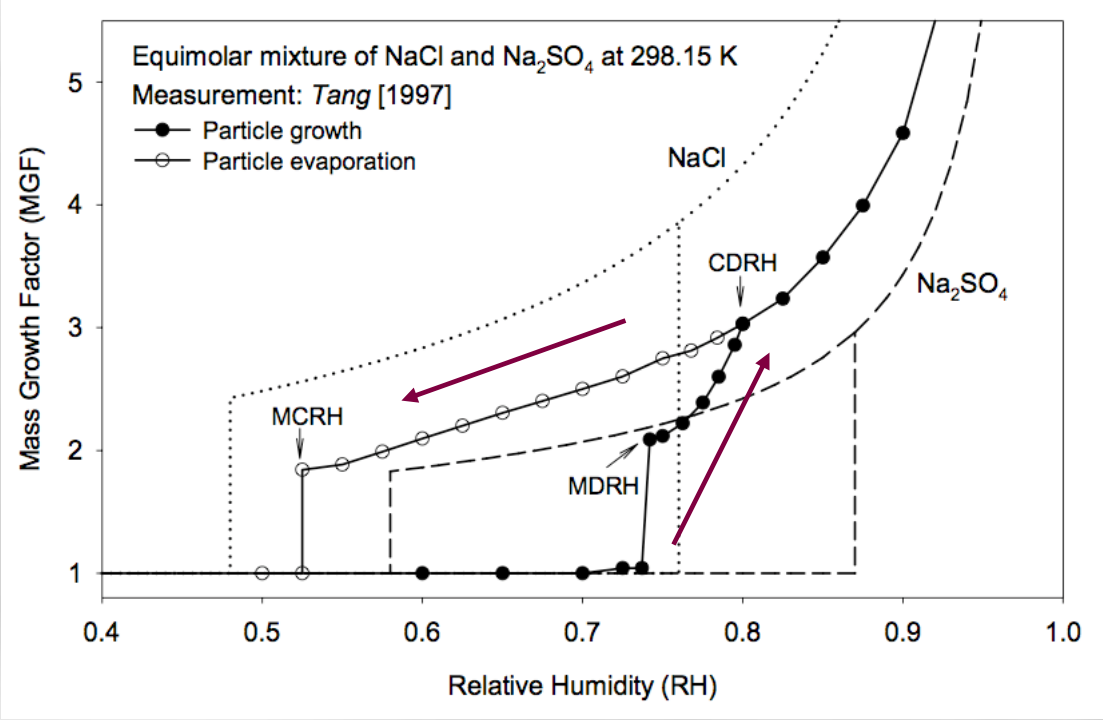


Many updates and bug fixes since version 2.1

Aerosol Chemistry (4)

Treatment of Aerosol Water in MOSAIC

- In a Lagrangian framework, relatively straight-forward to keep track of hydration history of aerosols, but …
- In an Eulerian framework, aerosols in different grid cells with different hydration histories can mix together
- All particles in a given bin are placed either on the lower or upper curve of hydration hysteresis loop, using transported variable W_{hyst}



A good treatment for aerosol water is needed since it has a profound effect on aerosol optical properties

Aerosol Optical Properties

General Description and Assumptions

size and number distribution
composition
aerosol water
→ refractive indices
→ Mie theory
→ layer optical depth, τ_λ
single scattering albedo, ω_o
asymmetry factor, g
→ shortwave radiation

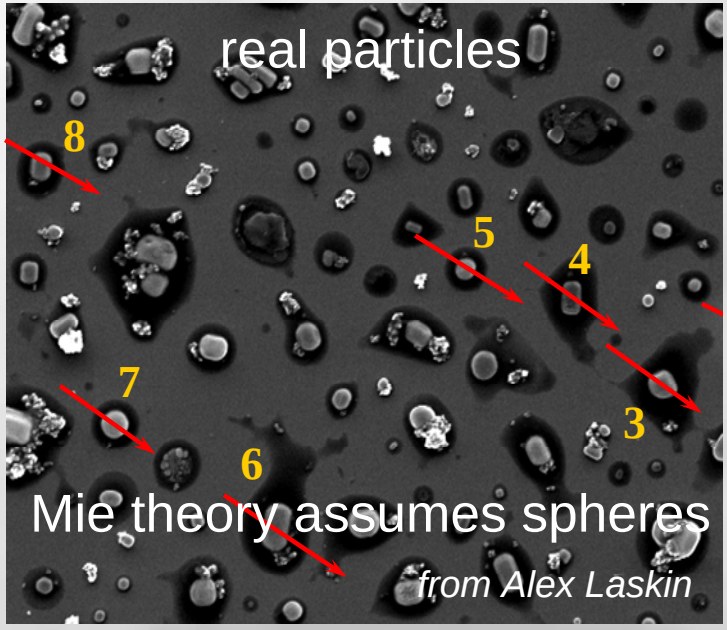
- **Volume averaging** approach to get refractive index
- τ, ω_o, and g function of wavelength, 300, 400 600, 1000 nm
- $\omega_o = k_s / (k_a + k_s)$, k_s and k_a = scattering and absorption coefficients
- This summer: **shell-core** approach to be implemented

Mass, composition, and size distribution:

more mass ➔ bigger radiative impact

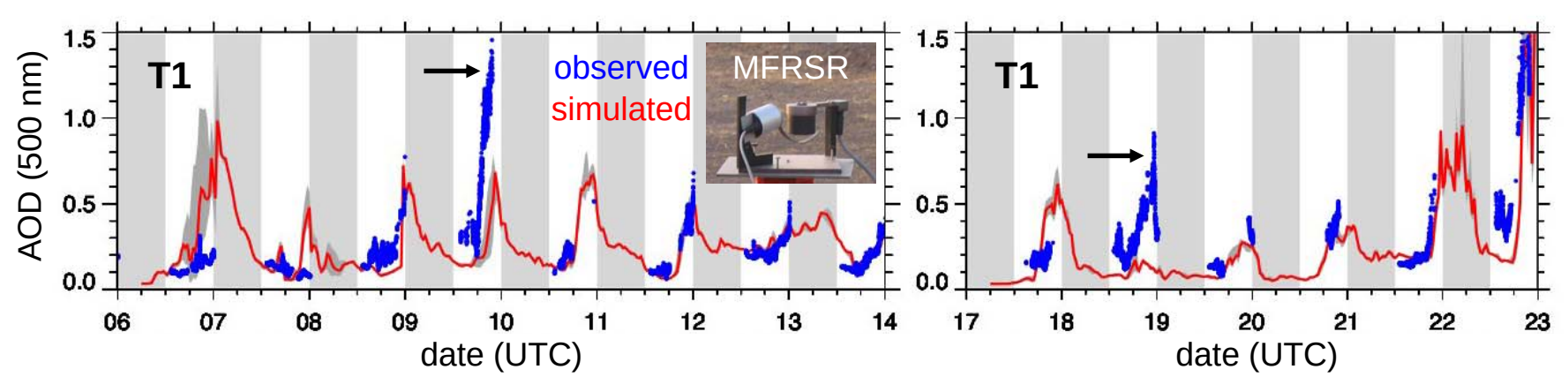
relative amount of black carbon ➔ k_s & k_a

largest effects near 0.4 m



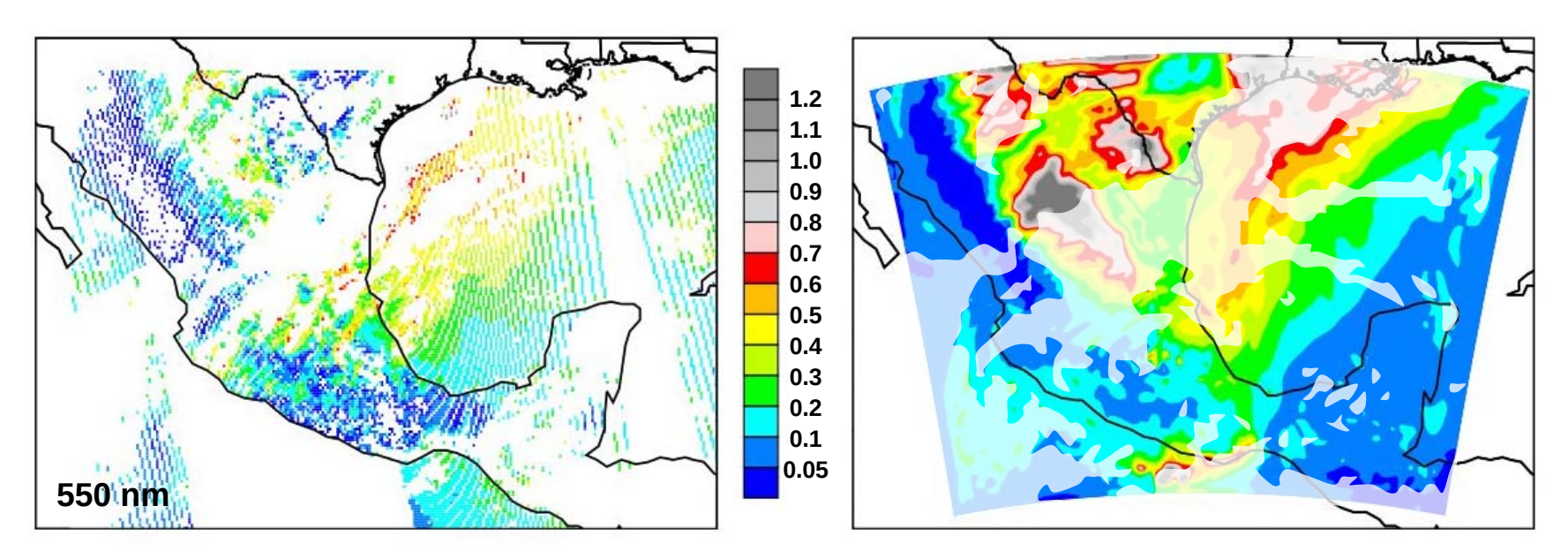
Observed vs Simulated AOD

AOD during March 2006 for MILAGRO Field Campaign



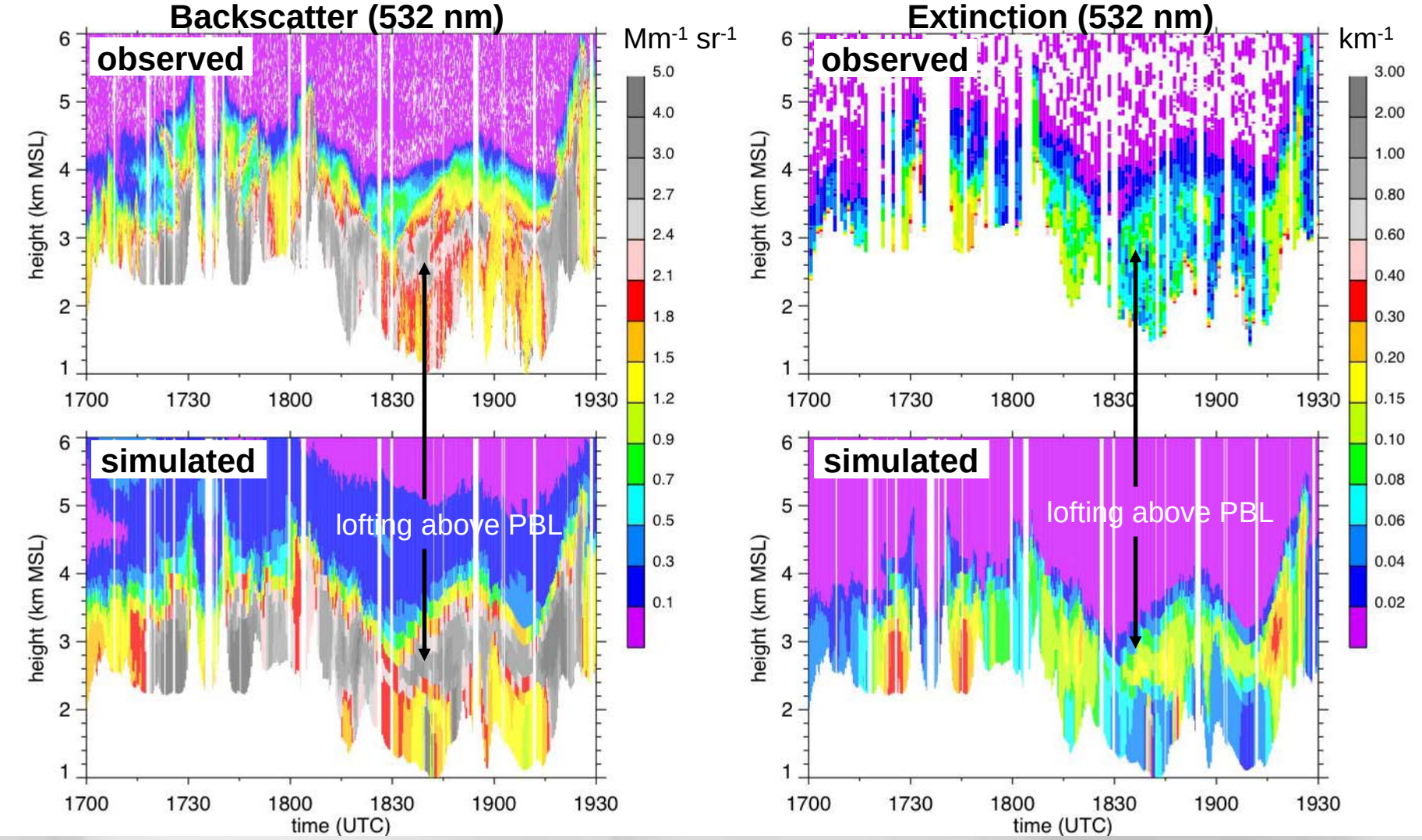
MODIS AOD, ~1930 UTC March 10

Simulated AOD, 20 UTC March 10



Observed Lidar vs Simulated

NASA B200 Aircraft Flight Path 13 March 2006 during MILAGRO



- Backscatter output not in released version of WRF-chem

Aerosol Direct Radiative Effects

General Description and Assumptions

size and number distribution
composition
aerosol water

→ refractive indices → Mie theory →

layer optical depth, τ_λ
single scattering albedo, ω_o
asymmetry factor, g

→ shortwave radiation

- Goddard shortwave scheme utilizes aerosol optical properties at 11 wavelengths, but the they are zero in default WRF / WRF-chem
- Use Angstrom relationship to interpolate between 4 wavelengths from optical property module to 11 wavelengths used in Goddard scheme
- Aerosols now account for scattering & absorption in Goddard scheme
- Effect of aerosols on longwave radiation not treated

Soon:

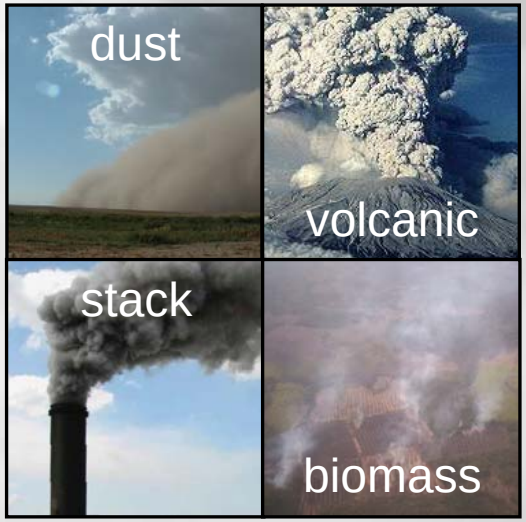
- Adapt CAM scheme (*ra_sw_physics = 3*) by replacing τ, ω_o, and g computed from off-line monthly averaged aerosols with on-line values
- Compute τ, ω_o, and g for MADE / SORGAM using a similar volume averaging approach employed by MOSAIC

Emissions

Treatment of Emissions Specific to CBM-Z or MOSAIC

Released Code:

- **Sea-Salt:** On-line computation based on 10-m speed and water cells (no distinction of fresh & salt water)



Not in Released Code (Preliminary):

- **Dust:** On-line computation based on u_*, soil type & moisture, land-use [*Shaw et al*., Atmos. Environ.]
- **Volcanic and Biomass Burning:** Add emission rates manually to anthropogenic files
- **Plume rise:** Based on on-line stability and stack parameters (T, D, V_e), but hard-coded

In Progress:

- **Biogenic:** Waiting for MEGAN [*Guenther et al.,* 2006] to be implemented in WRF-chem by C. Wiedinmyer (NCAR) and S. Chung (WSU) by July with species compatible with CBM-Z. *Bio_emiss_opt = 1* works (on-line computation), *but bio_emiss_opt = 2* (off-line computation) requires user input

Cloud-Aerosol Interactions (1)

Cloud Droplet Number

- converted Lin et al. microphysics scheme (*mp_physics=2*) to a two-moment treatment (mass & number)

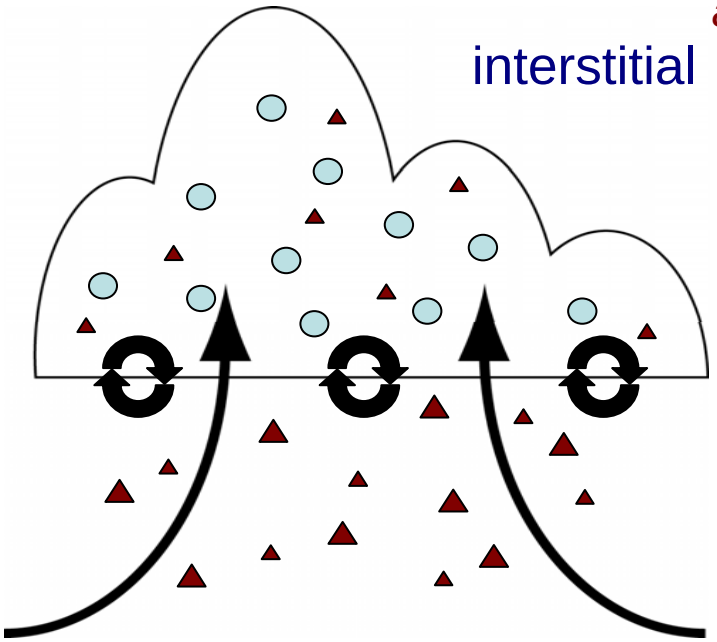
$$\frac{\partial N_k}{\partial t} = -(V \bullet \nabla N)_k + D_k - C_k - E_k + S_k$$

N_k - grid cell mean droplet number mixing ratio in layer k
D_k - vertical diffusion
C_k - droplet loss due to collision/coalescence & collection
E_k - droplet loss due to evaporation
S_k - droplet source due to nucleation

- cloud droplet number source determined by aerosol activation (for meteorology-only runs a prescribed aerosol size distribution is used)
- droplet number and cloud water mixing ratio used to compute effective cloud-particle size for computing cloud optical depth in Goddard shortwave radiation scheme (*ra_sw_physics=2*)

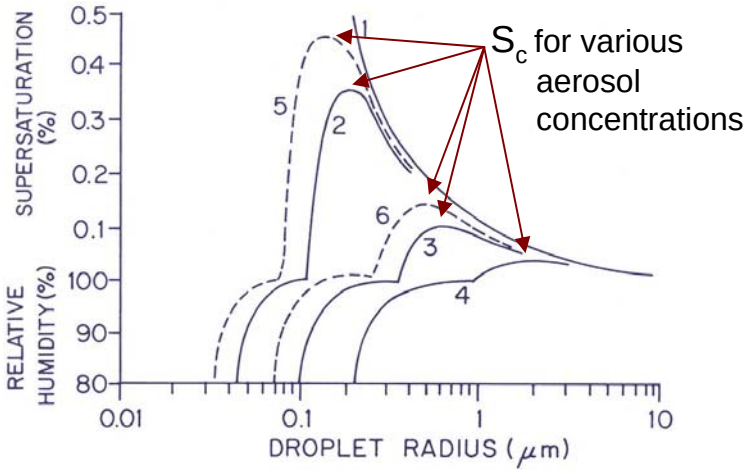
Cloud-Aerosol Interactions (2)

Activation and Resuspension



interstitial —*activation*→ cloud-borne —*resuspension*→ interstitial

Köhler Curves



Aerosol particles activated when the environmental supersaturation in the air "entering cloud", S, exceeds the aerosol particle's critical supersaturation, S_c

1: pure H_2O
2: 10^{-19} kg NaCl
3: 10^{-18} kg NaCl
4: 10^{-17} kg NaCl
5: 10^{-19} kg $(NH_4)SO_4$
6: 10^{-18} kg $(NH_4)SO_4$

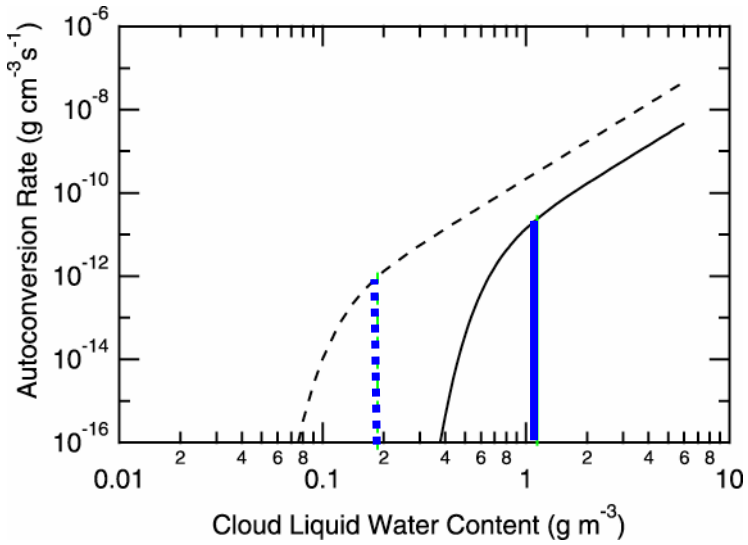
S_c, depends on aerosol size and composition

- interstitial and cloud-borne aerosol particles treated explicitly, doubling the number of transported species

Cloud-Aerosol Interactions (3)

Autoconversion

- autoconversion = coalescence of cloud droplets to form embryonic rain drops
- replaced autoconversion parameterization employed by Lin et al. microphysics (*mp_physics=2*) with *Liu et al.* [2005] parameterization
  - ➔ adds droplet number dependence
  - ➔ physically based w/o tunable parameters



Black: New Liu et al. parameterization
Blue: Kessler-type parameterization, similar to default Lin et al. scheme

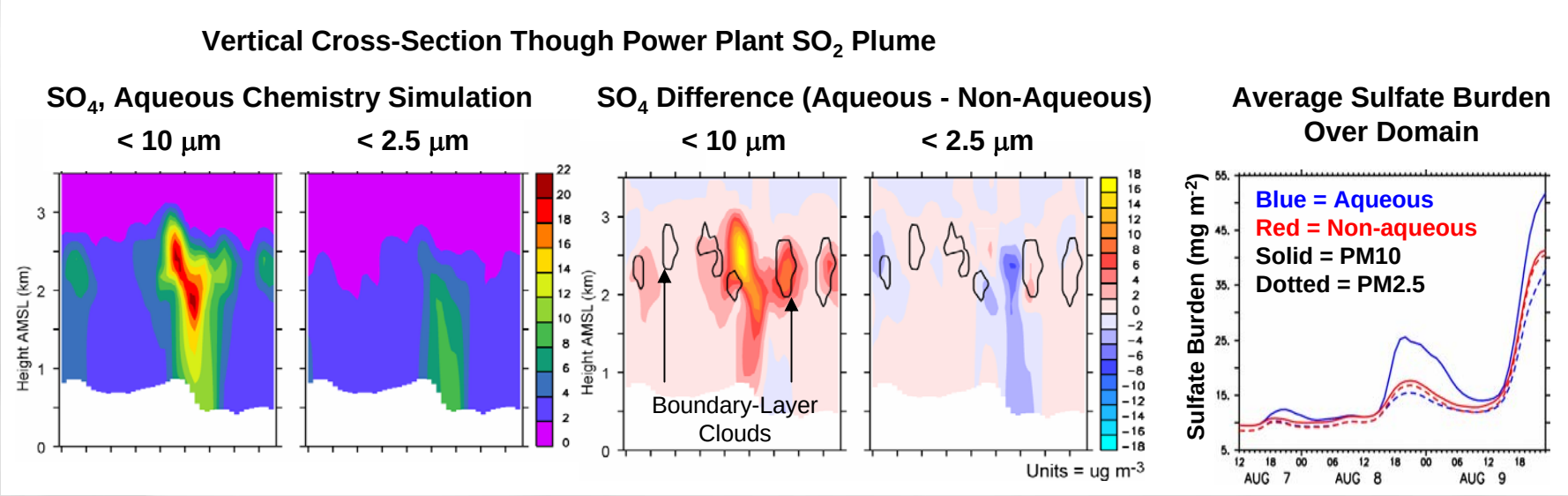
Dashed: N = 50 cm^{-3}
Solid: N = 500 cm^{-3}

Adapted from Fig. 3, Liu et al., 2005, GRL.

Cloud-Aerosol Interactions (4)

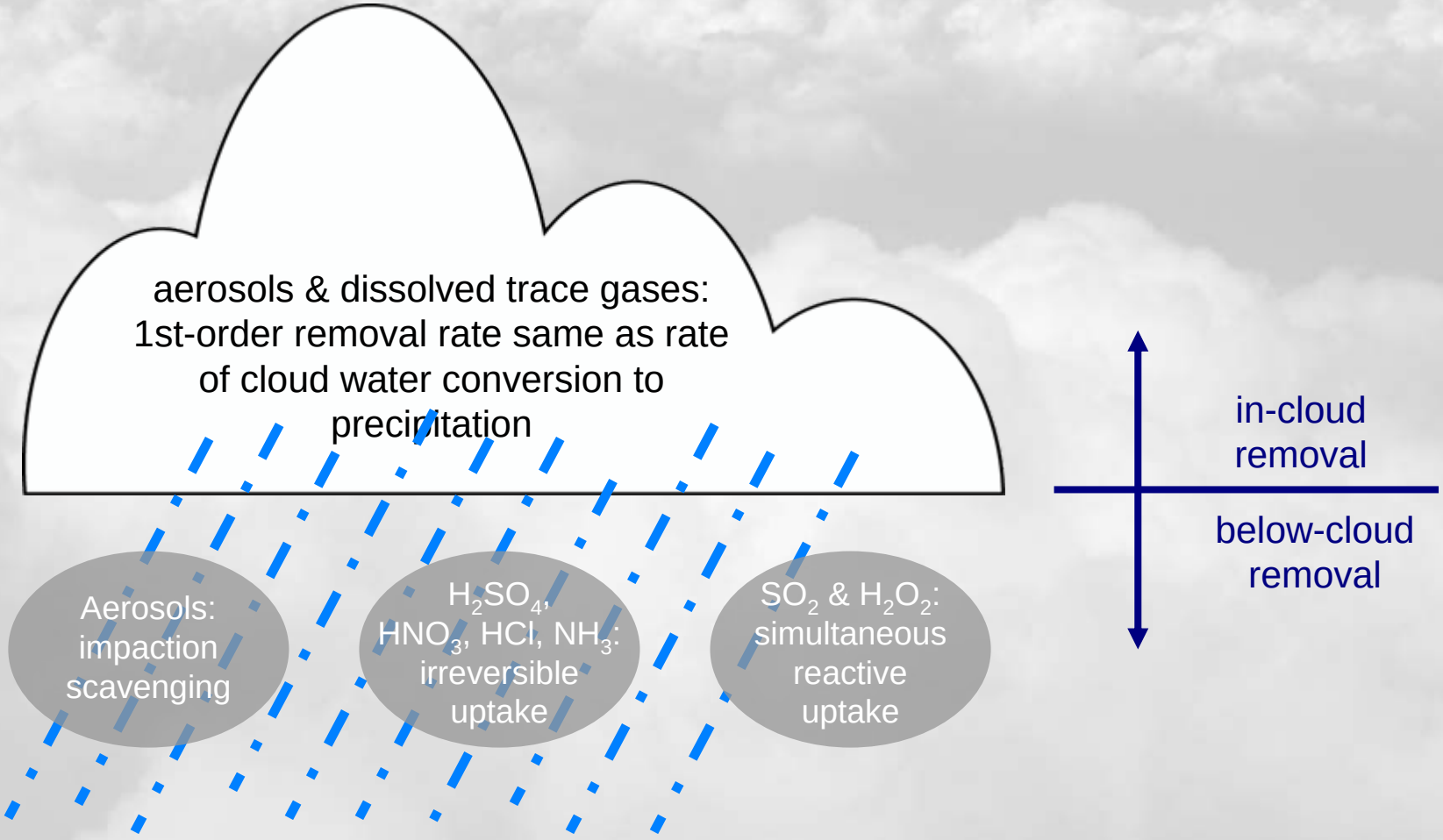
Aqueous Chemistry

- Bulk cloud-chemistry module of *Fahey and Pandis* [2001☐]
- Oxidation of S(IV) by H_2O_2, O_3, trace metals, and radical species
- Non-reactive uptake of HNO_3, HCl, NH_3, and other trace gases
- Bulk mass changes partitioned among cloud-borne aerosol size bins, followed by transfer of mass & number between bins due to growth



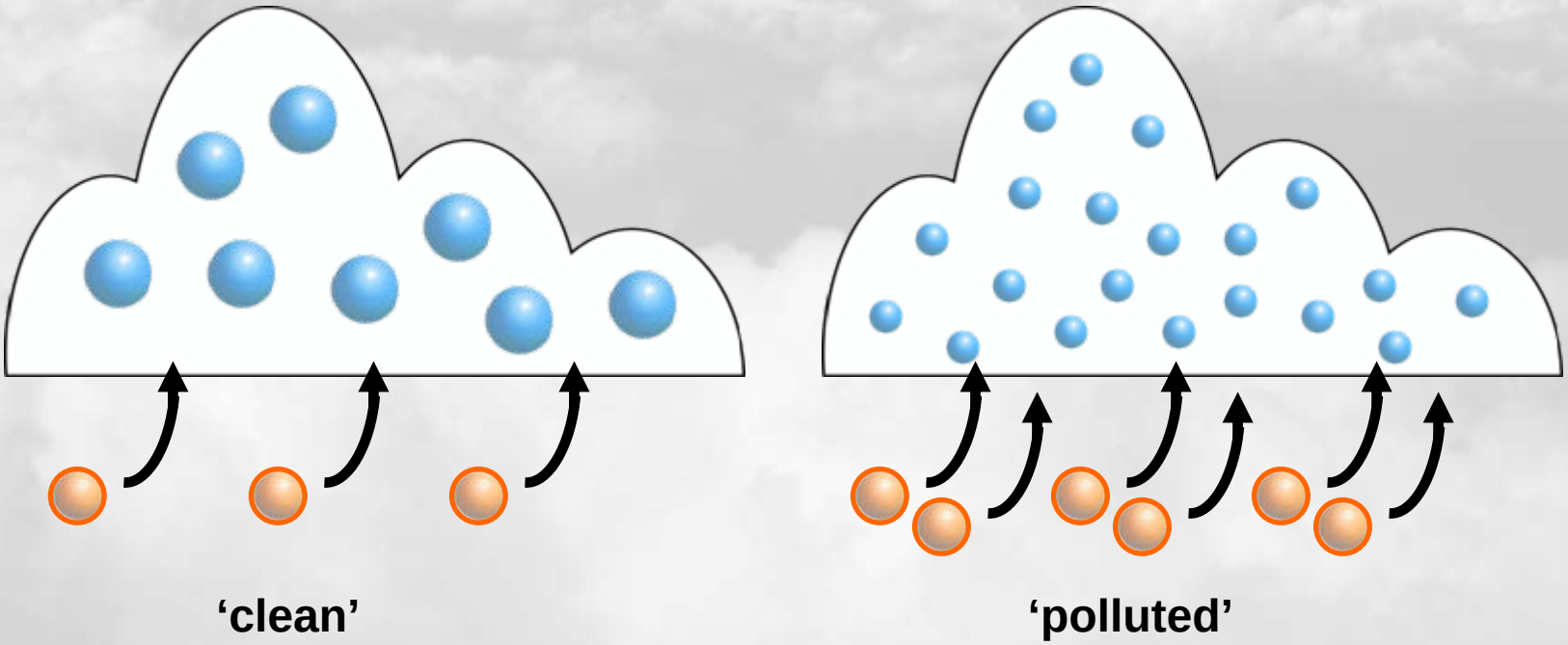
Cloud-Aerosol Interactions (5)

Scavenging



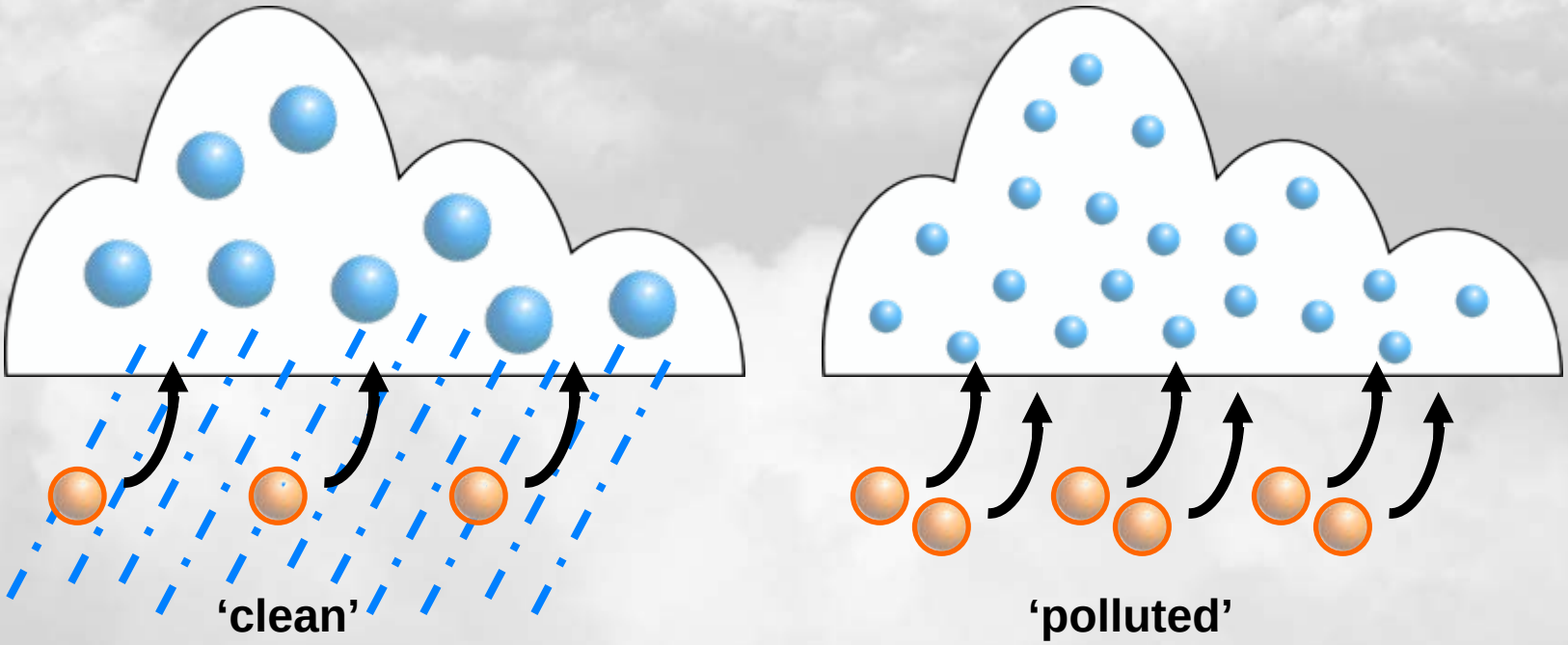
scavenged aerosols and gases are assumed
to be instantly removed (wet deposited)

First Indirect Effect



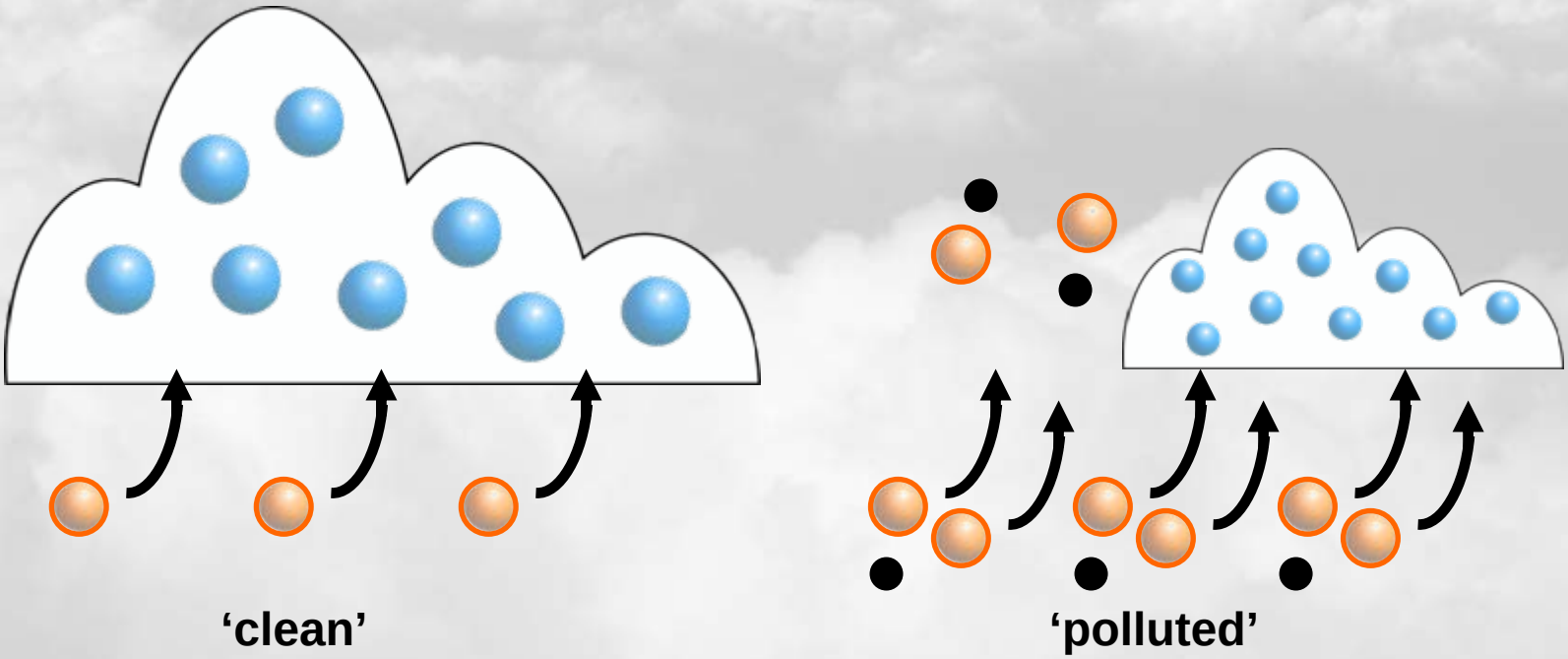
- Influence of cloud optical depth through impact on effective radius, with no change in water content of cloud

Second Indirect Effect



- Influence of cloud optical depth through influence of droplet number on mean droplet size and hence initiation of precipitation

Semi-Direct Effect



- Influence of aerosol absorption of sunlight on cloud liquid water and hence cloud optical depth

Interactions Not-Treated

- **First Dispersion Effect:** Influence on cloud optical depth through influence of aerosol on dispersion of droplet size distribution, with no change in water content of cloud
- **Second Dispersion Effect:** Influence on cloud optical depth through influence of aerosol on dispersion and hence initiation of precipitation
- **Glaciation Indirect Effect:** Influence of aerosol on conversion of haze and droplets to ice crystals, and hence on cloud optical depth and initiation of precipitation