

Aerosol Direct and Indirect Forcing

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WRF-Chem Tutorial, July 18, 2011, Boulder CO

Background

First A Brief History ...

- Gas-phase and aerosol models were implemented first in WRF-Chem
- Aerosol-radiation-cloud interactions were added to MOSAIC aerosol model, adapted from those used in global climate model
- Then, aerosol-radiation-cloud interactions coupled with GOCART and MADE/SORGAM
- We are currently adding more capabilities, making modules more generic, and trying to follow WRF coding guidelines

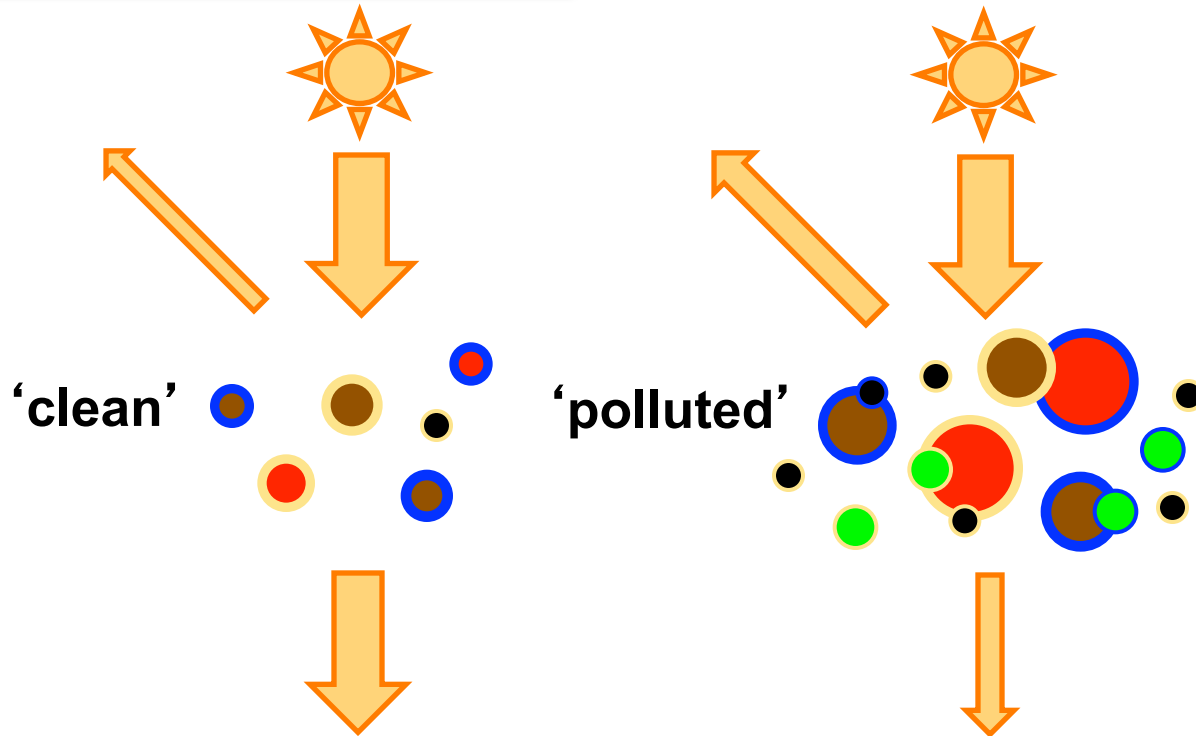
Our overall motivation is to use the model to better understand and parameterize local to regional-scale evolution of particulates and their effect on radiation, clouds, and chemistry

Discuss Aerosol-Radiation-Cloud Interactions Treated in WRF

- Part 1: Direct Effects
- Part 2: Indirect Effects



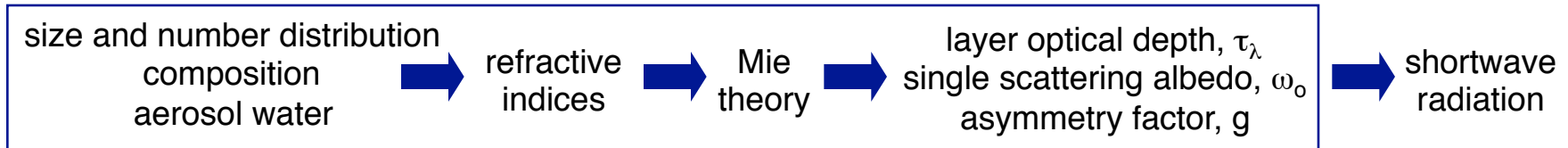
Part 1: Aerosol Direct Effects



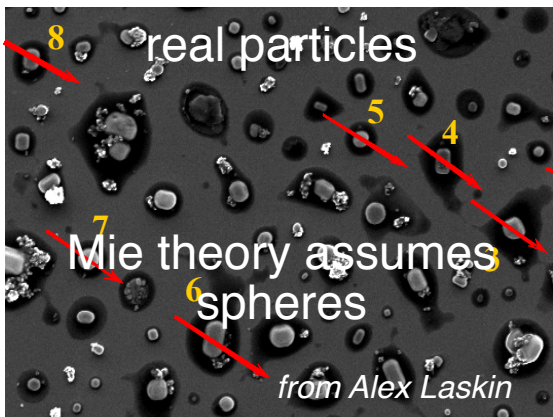
What are the impacts of altering the radiation budget on meteorology?

Aerosol Optical Properties

General Description and Assumptions



- τ , ω_o , and g function of wavelength, 300, 400, 600, 1000 nm
 - $\tau = \text{TAUAER1}, \text{TAUAER2}, \text{TAUAER3}, \text{TAUAER4}$
 - $\omega_o = \text{WAER1}, \text{WAER2}, \text{WAER3}, \text{WAER4}$
 - $g = \text{GAER1}, \text{GAER2}, \text{GAER3}, \text{GAER4}$
- } registry.chem
- In some parts of the code (/phys), TAUAER1 called TAUAER300, etc.,
 - $\omega_o = k_s / (k_a + k_s)$, k_s and k_a = scattering and absorption coefficients
 - various methods of obtaining refractive index



Mass, composition, and size distribution:

- more mass ➔ bigger radiative impact
- amount of black carbon ➔ k_a
- aerosol size ➔ k_s



Aerosol Direct Radiative Effects

General Description and Assumptions



- Goddard shortwave scheme utilizes aerosol optical properties at 11 wavelengths, but they are zero in default WRF
- Code added to Goddard scheme that uses Angstrom relationship to interpolate between 4 wavelengths from optical property module to 11 wavelengths
- Aerosols now account for scattering & absorption in Goddard scheme

New in Version 3.3

Coupling Aerosols to RRTMG Shortwave and Longwave Scheme

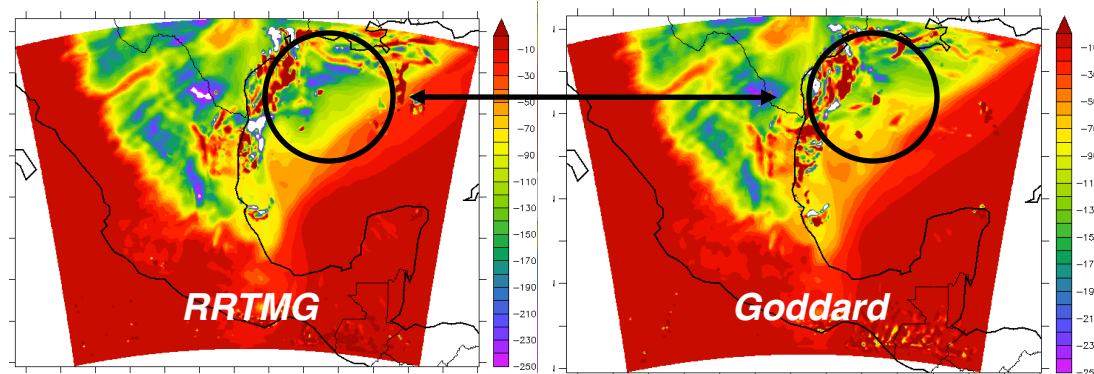


Utilize same code, but now arrays needed for longwave radiation added

see Zhao et al., ACP, 2010 for more details

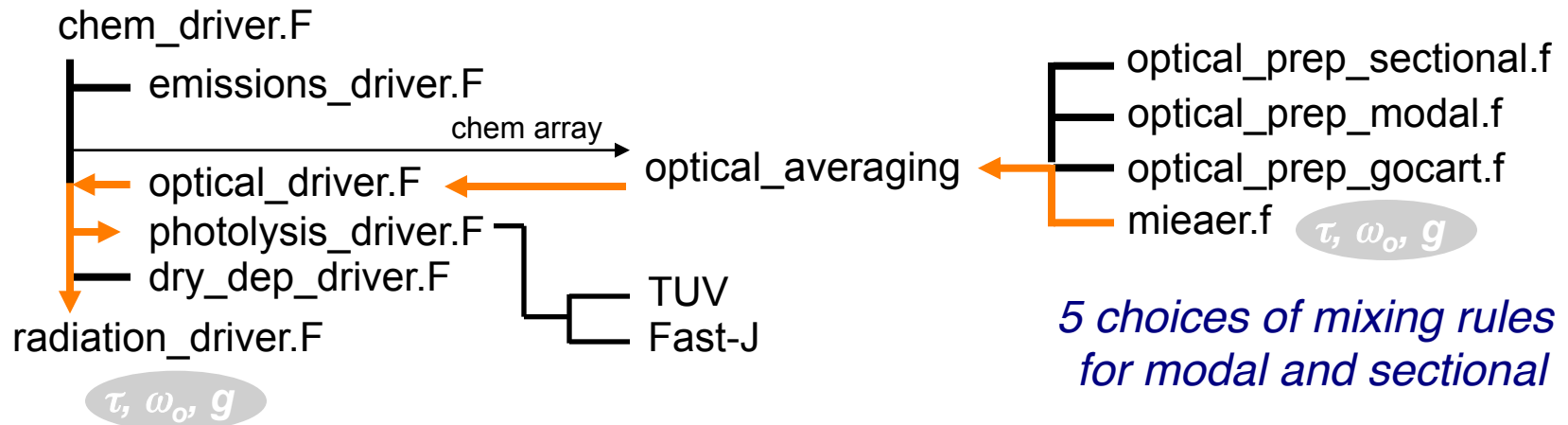
- In addition to previous arrays for τ , ω_0 , and g , now have τ for longwave radiation, TAUAERLW1 – 16 (16 wavelengths)
- Local arrays TAUAERSW = TAUAER, WAERSW = WAER, GAERSW = GAER
- Tests show impact of aerosols very similar for two radiation schemes

difference in SW due to aerosols



Coding Structure

Generic Aerosol Optical Properties Modules for WRF-Chem

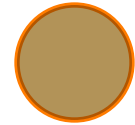


Example of making the code more generic and interoperable – want to have optical property computations in one place rather than in each aerosol model

Choice of Mixing Rule

- **Volume Averaging**

- averaging of refractive indices based on composition



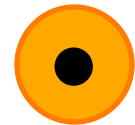
- **Maxwell-Garnett** [*Borhren and Huffman, 1983*]

- small spherical randomly distributed in particle



- **Shell-Core** [*Ackermann and Toon, 1983; Borhren and Huffman, 1983*]

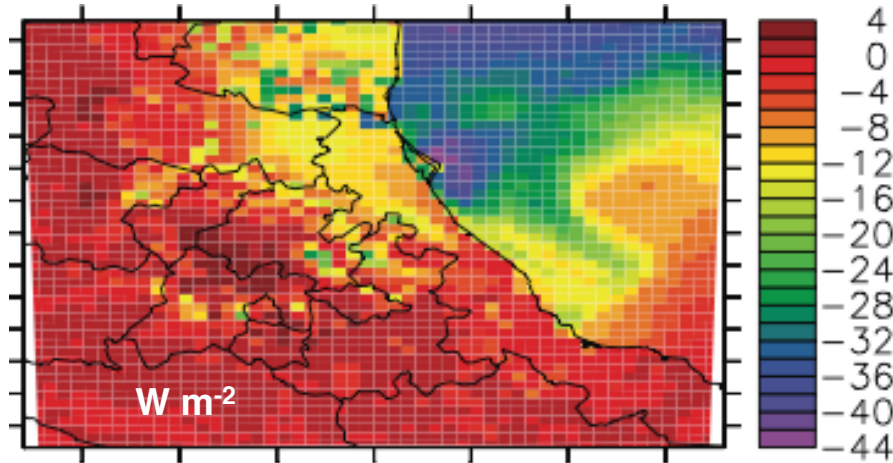
- black carbon core and average of other compositions in shell



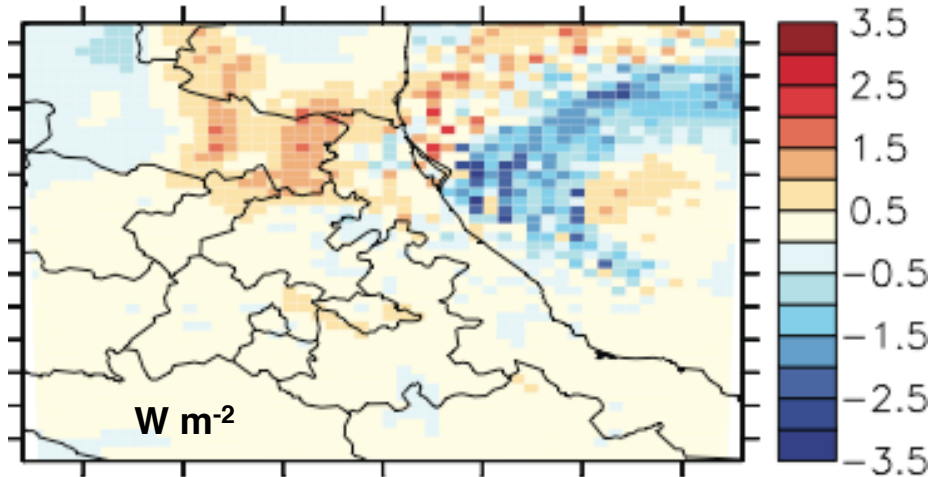
- Volume-Averaging and Maxwell-Garnett computed either exactly or approximately (faster)
- Shell-core the most expensive computationally, but presumably the most accurate
- All very sensitive to changes in the amount of black carbon
- *aer_op_opt* in namelist.input:
 - 1 = Volume-Averaging approximate
 - 2 = Maxwell-Garnett approximate
 - 3 = Volume-Averaging exact
 - 4 = Maxwell-Garnett exact
 - 5 = Shell-Core

Mie Calculation Accuracy

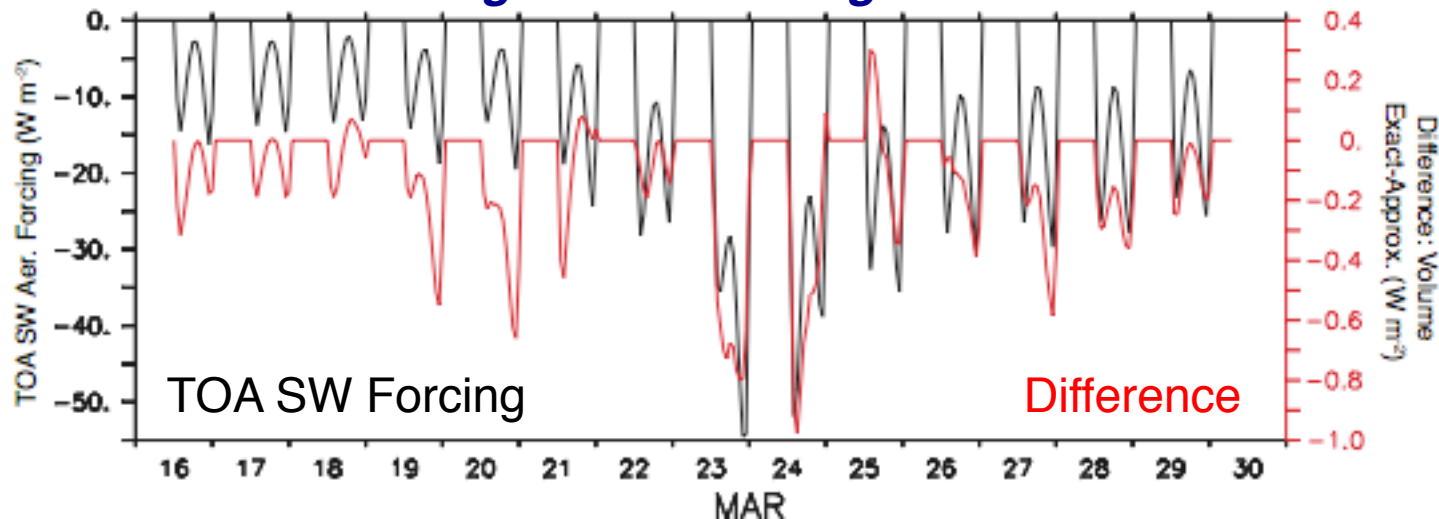
Aerosol Effect on Shortwave TOA



Difference: Exact - Approximate



Average over Modeling Domain



Assumptions

- Interfaces with GOCART, MADE/SORGAM, and MOSAIC, but linking to other aerosol models should be relatively easy

- **Sectional (MOSAIC):** tested only with 4 and 8 size bins – should work if additional size bins are specified

PNNL

- **Modal (MADE/SORGAM):** divides mass in modes into 8 sections - could divide into more sections to be more accurate

PNNL

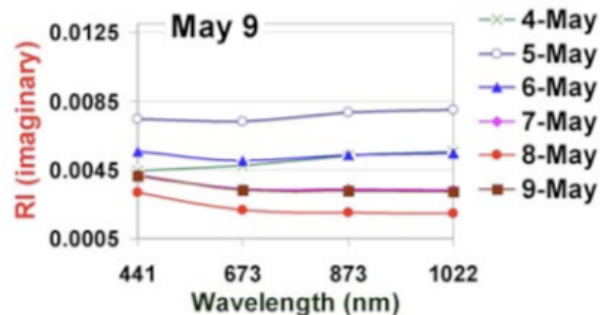
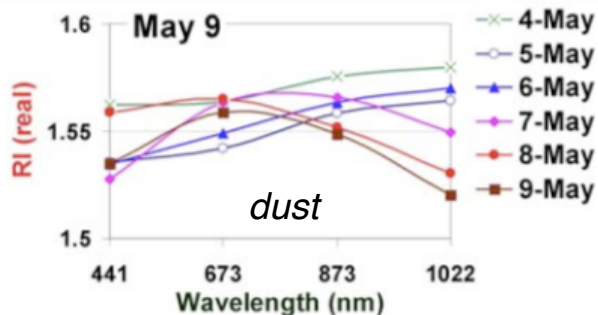
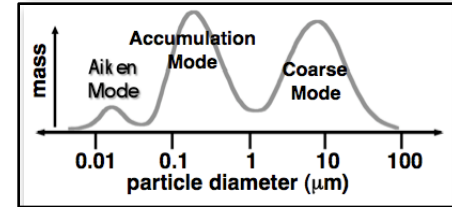
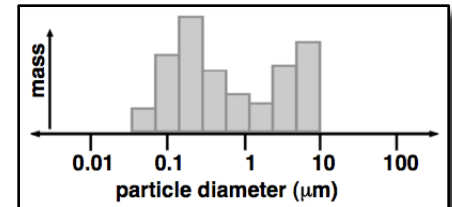
- **Bulk (GOCART):** converts bulk mass into assumed modal distribution, then divides mass into 8 sections

NOAA

- Refractive indices may need updating

- Range of values reported in the literature

- Wavelength dependence of refractive indices for some species **New in V3.3**

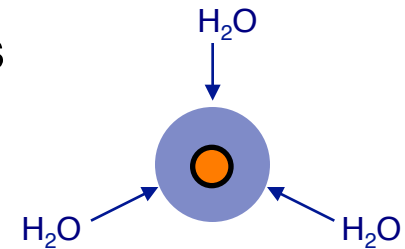


Dust refractive indices for SW constant by default – need to modify code to turn on

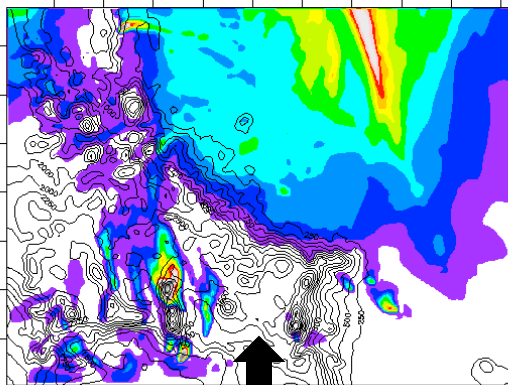
from Prasad and Singh, JGR, 2007

Importance of Aerosol Water

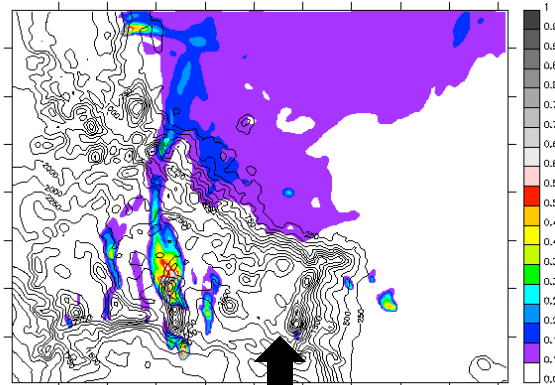
- Aerosol water will have a big impact on optical properties
- Aerosol water depends on relative humidity (RH); thus, predictions of RH need to be monitored when evaluating aerosol direct radiative forcing



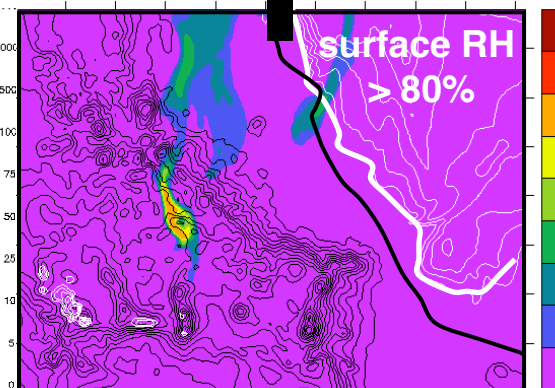
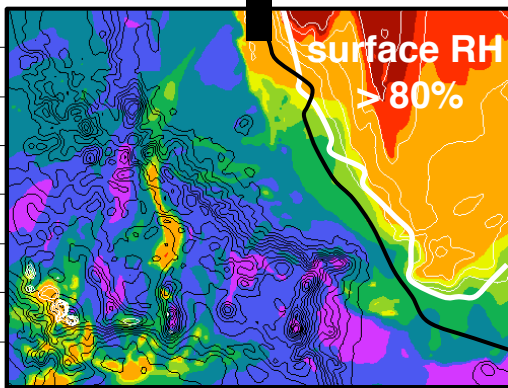
AOD: MOSAIC



AOD: MADE / SORGAM



Aerosol Water Column

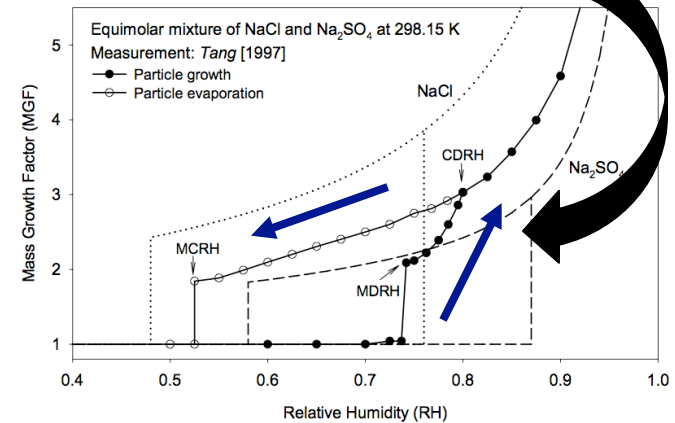


Aerosol Water

GOCART: diagnosed from RH using *Petters and Kreidenweiss [2007]*

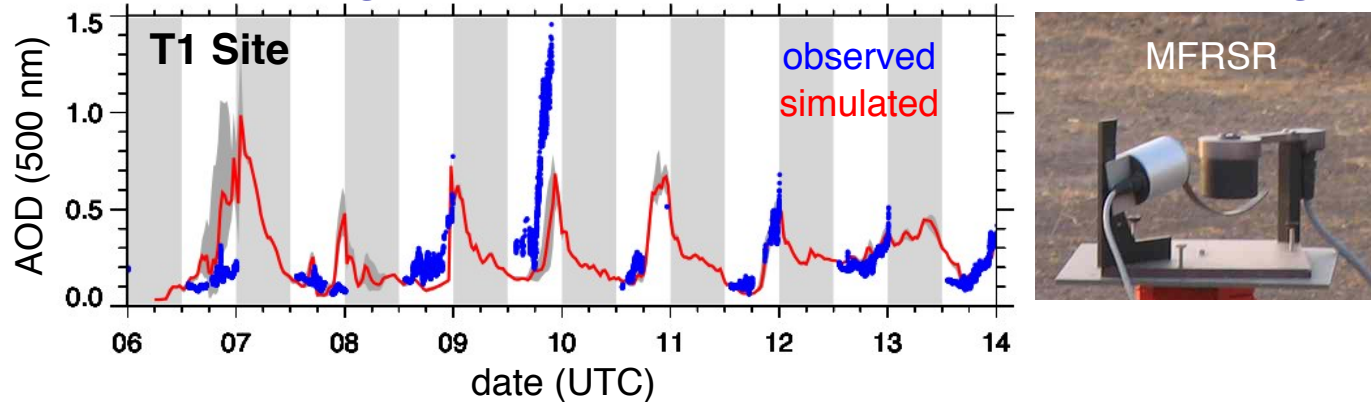
MADE / SORGAM: diagnosed

MOSAIC: prognostic specie that accounts for hysteresis effect

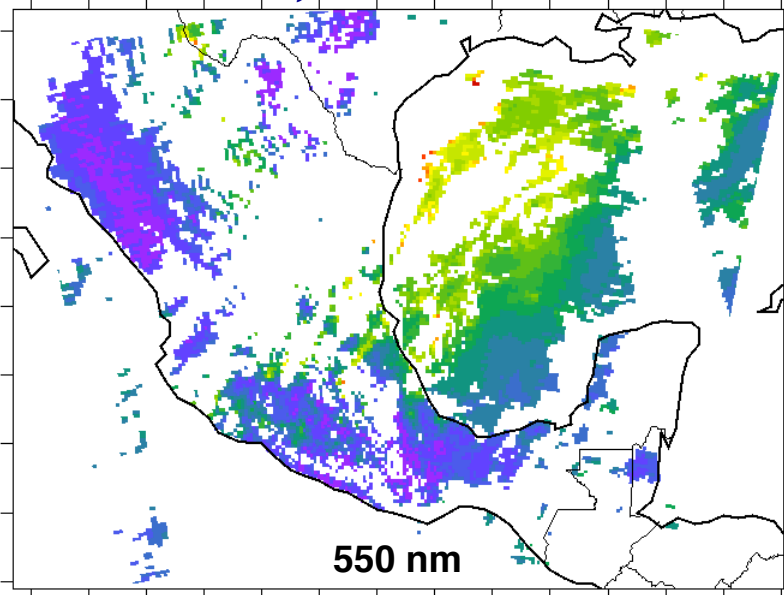


Example 1: Aerosol Optical Depth

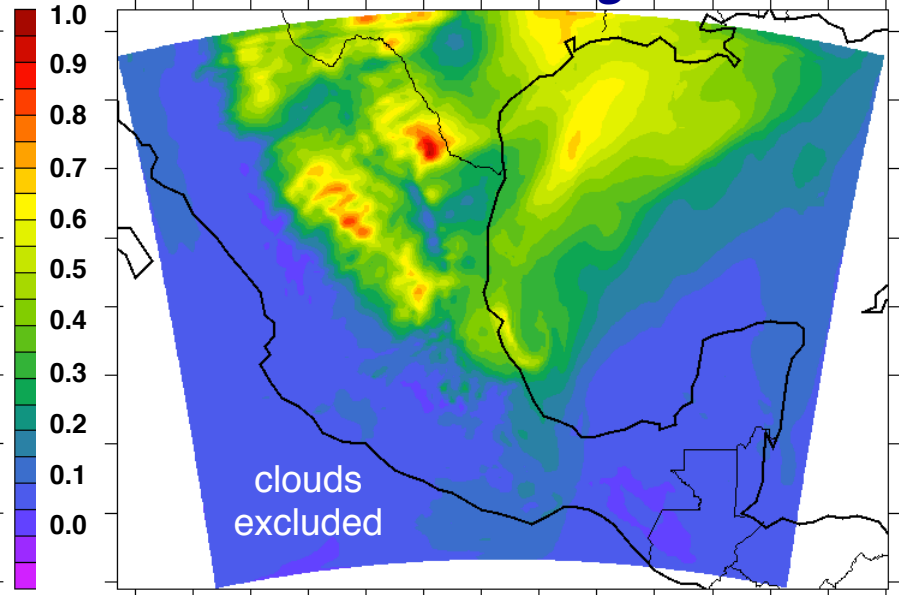
AOD during March 2006 for MILAGRO Field Campaign



MODIS AOD, ~1930 UTC March 10



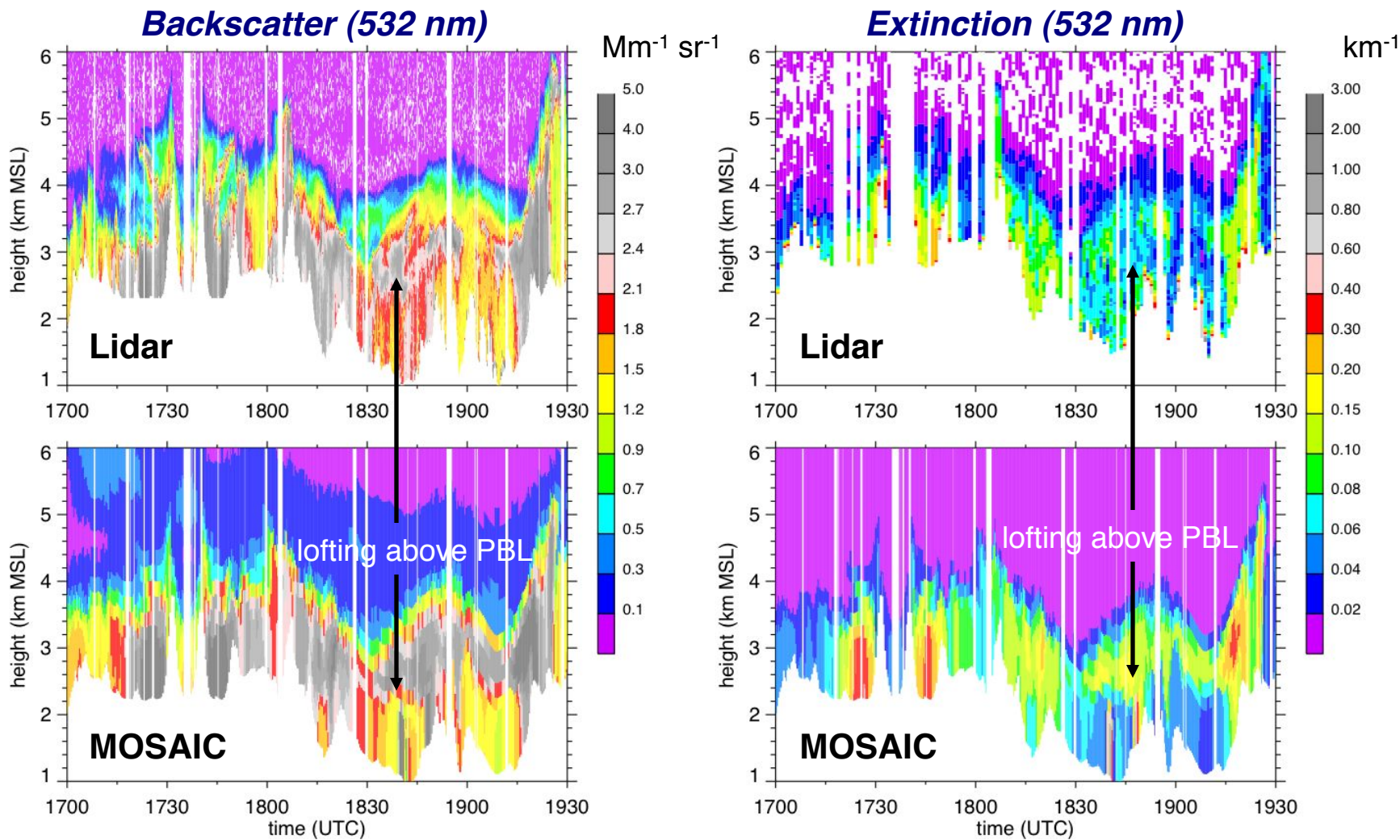
Simulated AOD using MOSAIC



Use Angstrom Exponent to get values at 550 nm from 500 and 600 nm computations

Example 2: Backscatter and Extinction Profiles

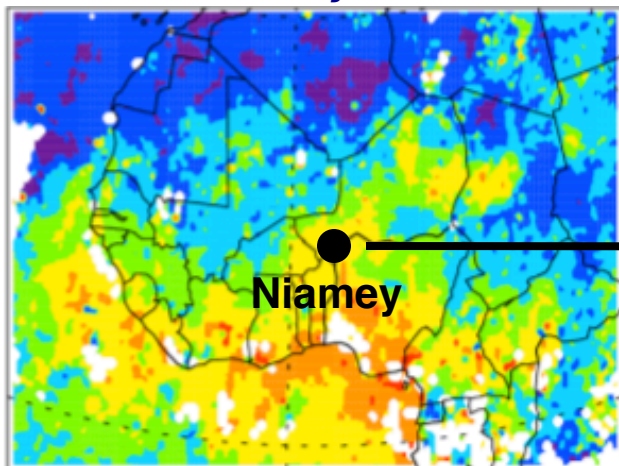
NASA B200 Aircraft Flight Path 13 March 2006 during MILAGRO



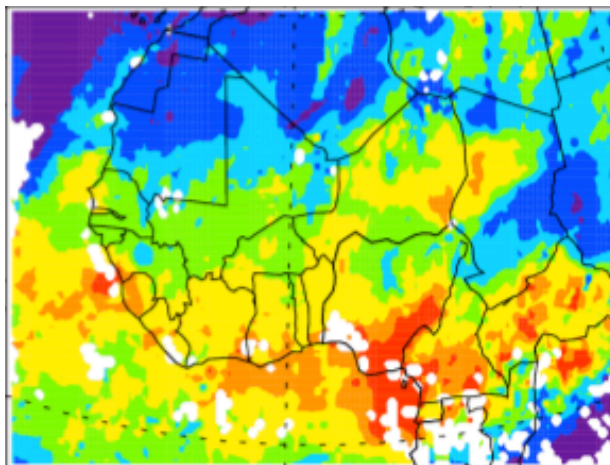
Use Angstrom Exponent to get values at 550 nm from 500 and 600 nm computations

Example 3: Radiative Heating Rate

Averaged Terra-MISR AOD
January 2006

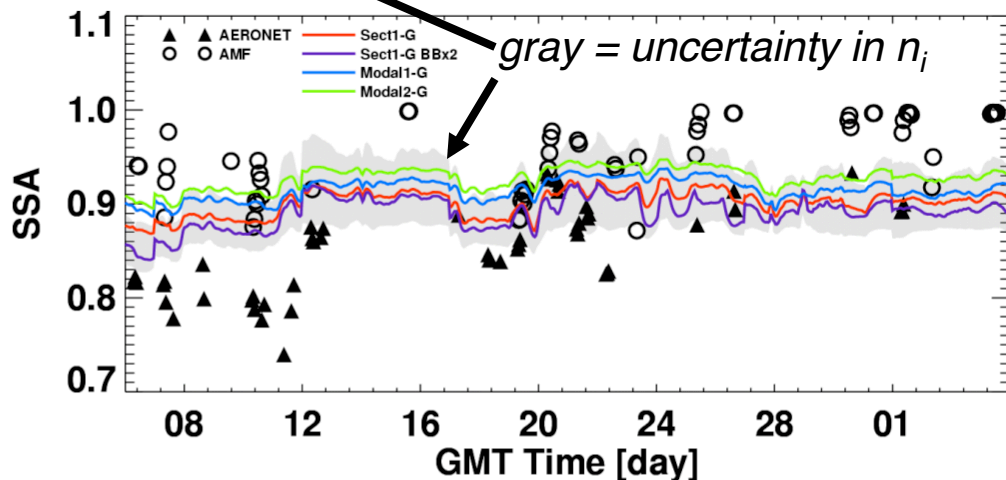
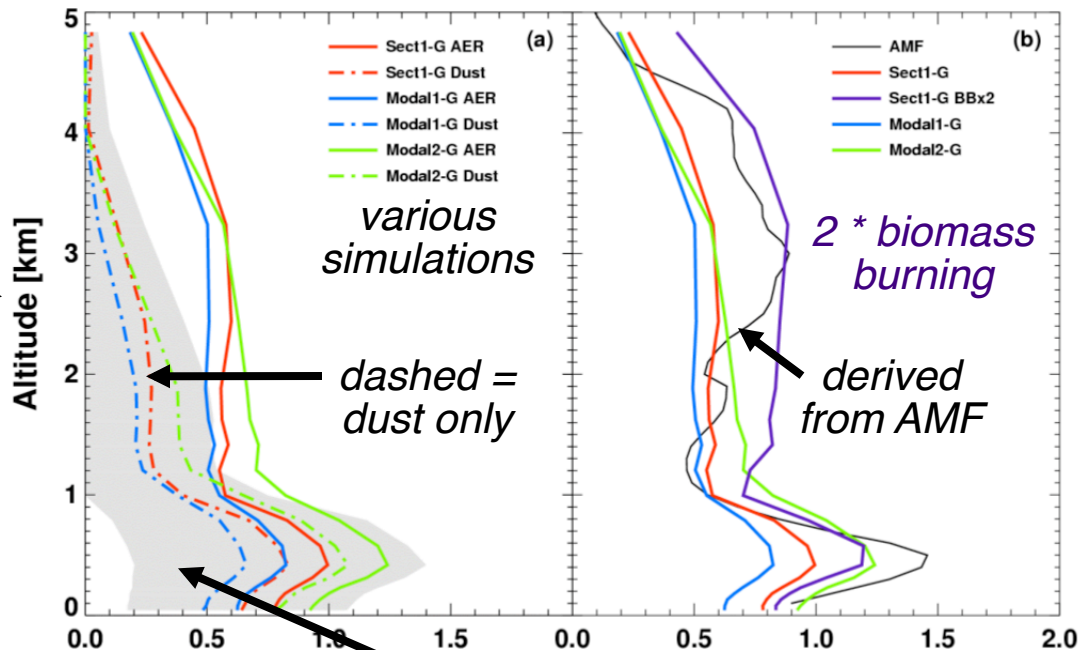


Simulated AOD
MOSAIC + GOCART dust



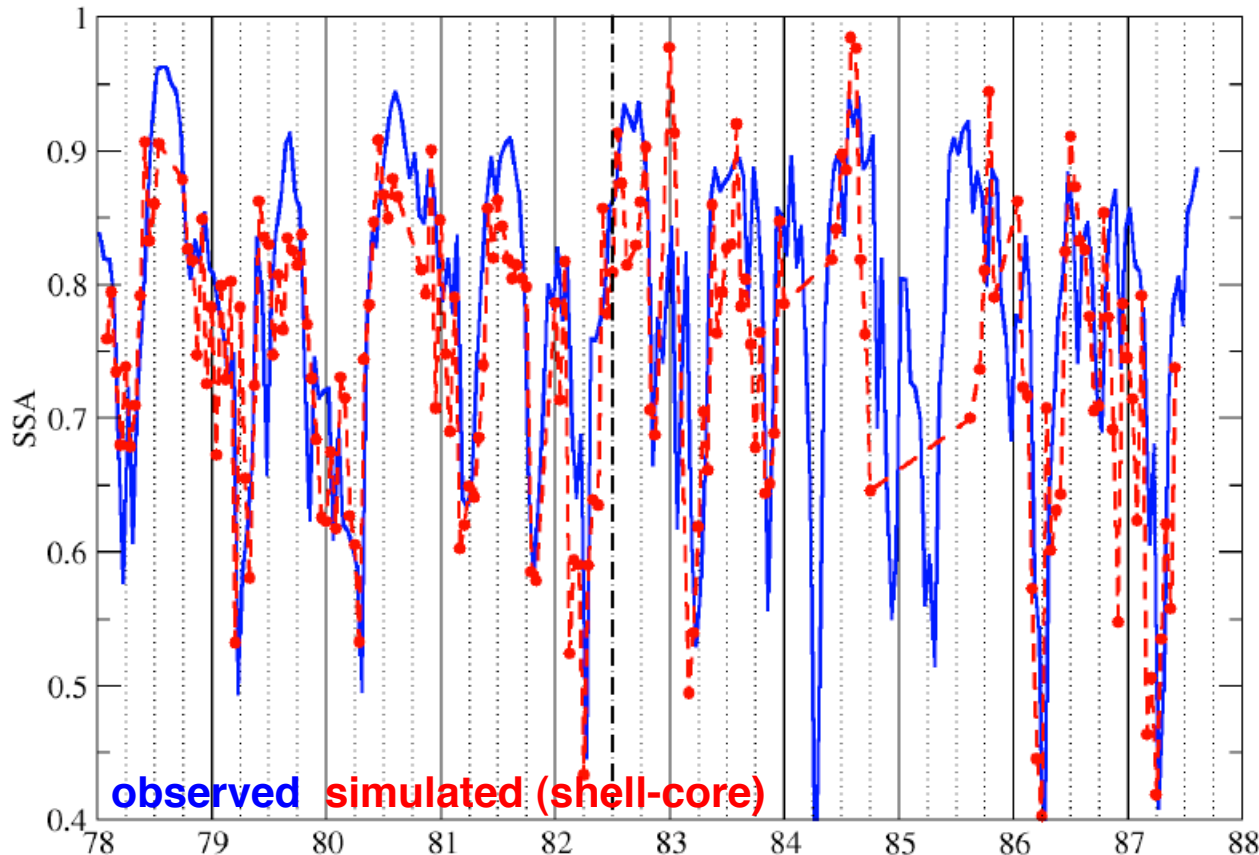
from Zhao et al., ACP, 2010

SW Radiative Heating Rate Profile ($K day^{-1}$)



Example 4: *Single Scattering Albedo*

SSA during March 2006 MILAGRO Field Campaign



Aerosol optical property modules driven by measurements of particulate mass, composition, and size distribution (some uncertainties in data)

Most of the error in scattering

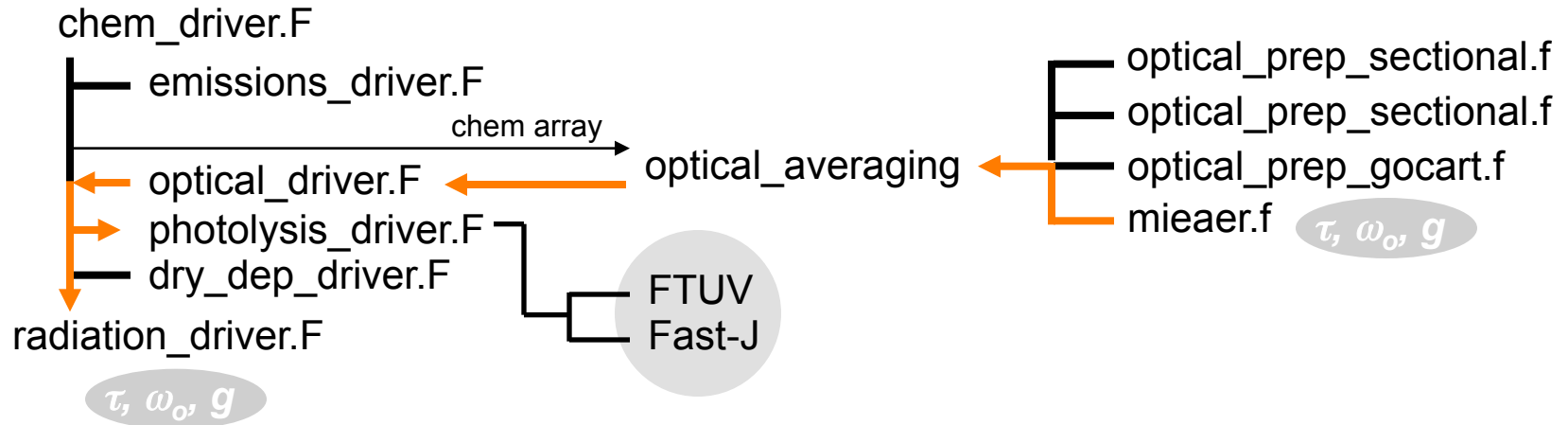
Other mixing rules obtain similar results

From offline version of aerosol optical property modules in WRF-chem, *Barnard et al. ACP, 2010*

Photolysis Rates

Aerosols → Photolysis Rates → Photochemistry

but clouds, if present, will have a bigger impact on photolysis rates than aerosols



- Fast-J: uses τ , ω_0 , and g computed by module_optical_averaging.F
 - *Note: limited testing of effect of aerosols on photolysis rates*
- FTUV: uses its own method of accounting for effects of aerosols on photolysis rates based on MADE/SORGAM species only
 - *MOSAIC aerosols will not affect photolysis rates when FTUV is used*



“fixing” this is not trivial – has not been a high priority

Settings in namelist.input

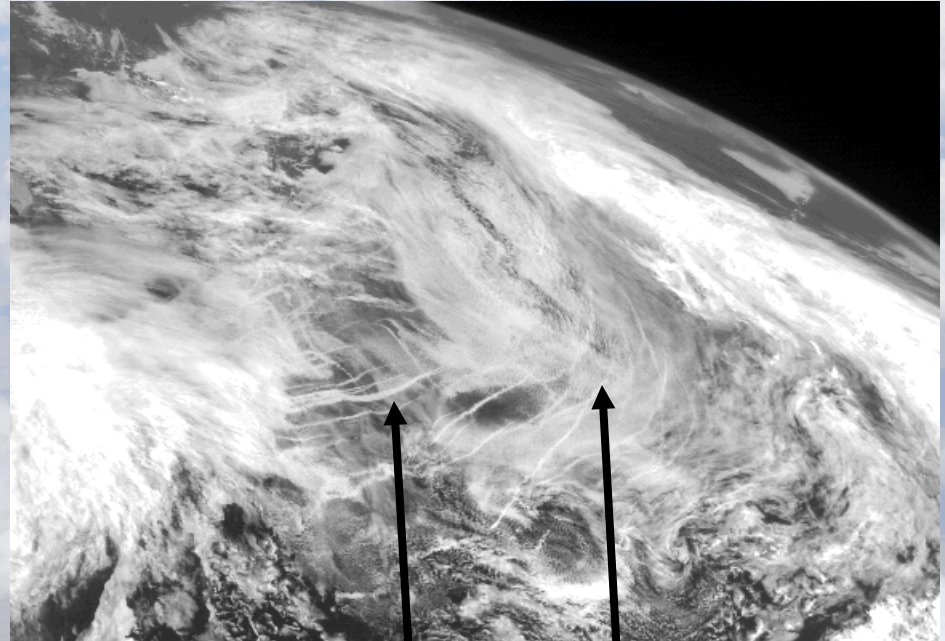
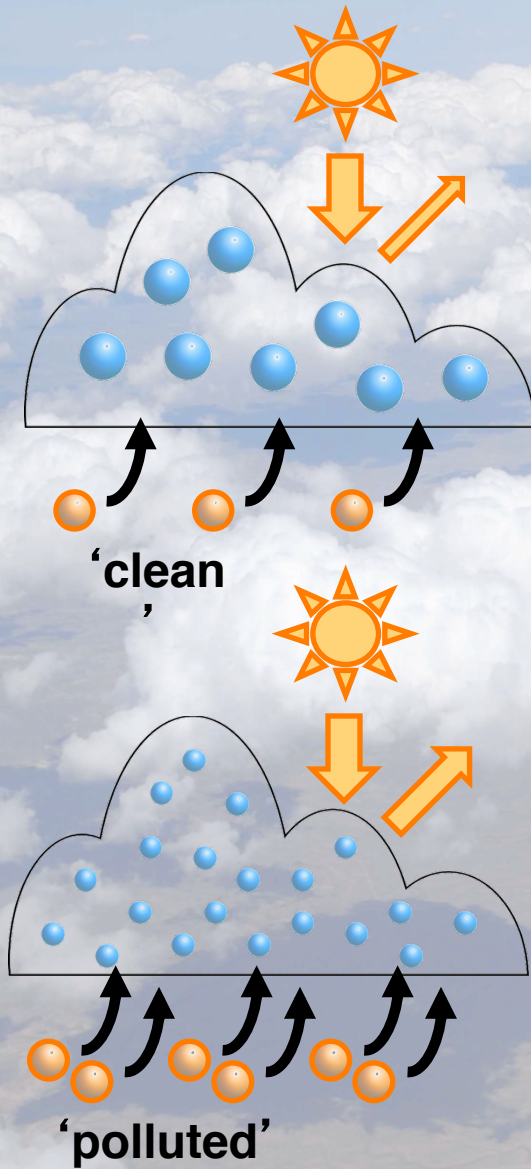
- $ra_sw_physics = 2$ - affects radiation computed by Goddard scheme
- $ra_sw_physics = 4$
- $ra_lw_physics = 4$ } affects radiation computed by RRTMG scheme
- $aer_ra_feedback = 1$, turns on aerosol radiation feedback
- $aer_op_opt = > 0$, define the mixing rule for Mie calculations
- Works similarly for GOCART, MADE/SORGAM, and MOSAIC options

Research – Possibly in Upcoming Releases of WRF:

- Different refractive indices for POA and SOA
 - *TOTOA now used in code, but could be divided into POA and SOA*
- More computationally efficient Mie calculations
- Mie routine that handles non-spherical particles
- Code to handle aerosol model with external mixtures



Part 2: Aerosol Indirect Forcing



ship-tracks

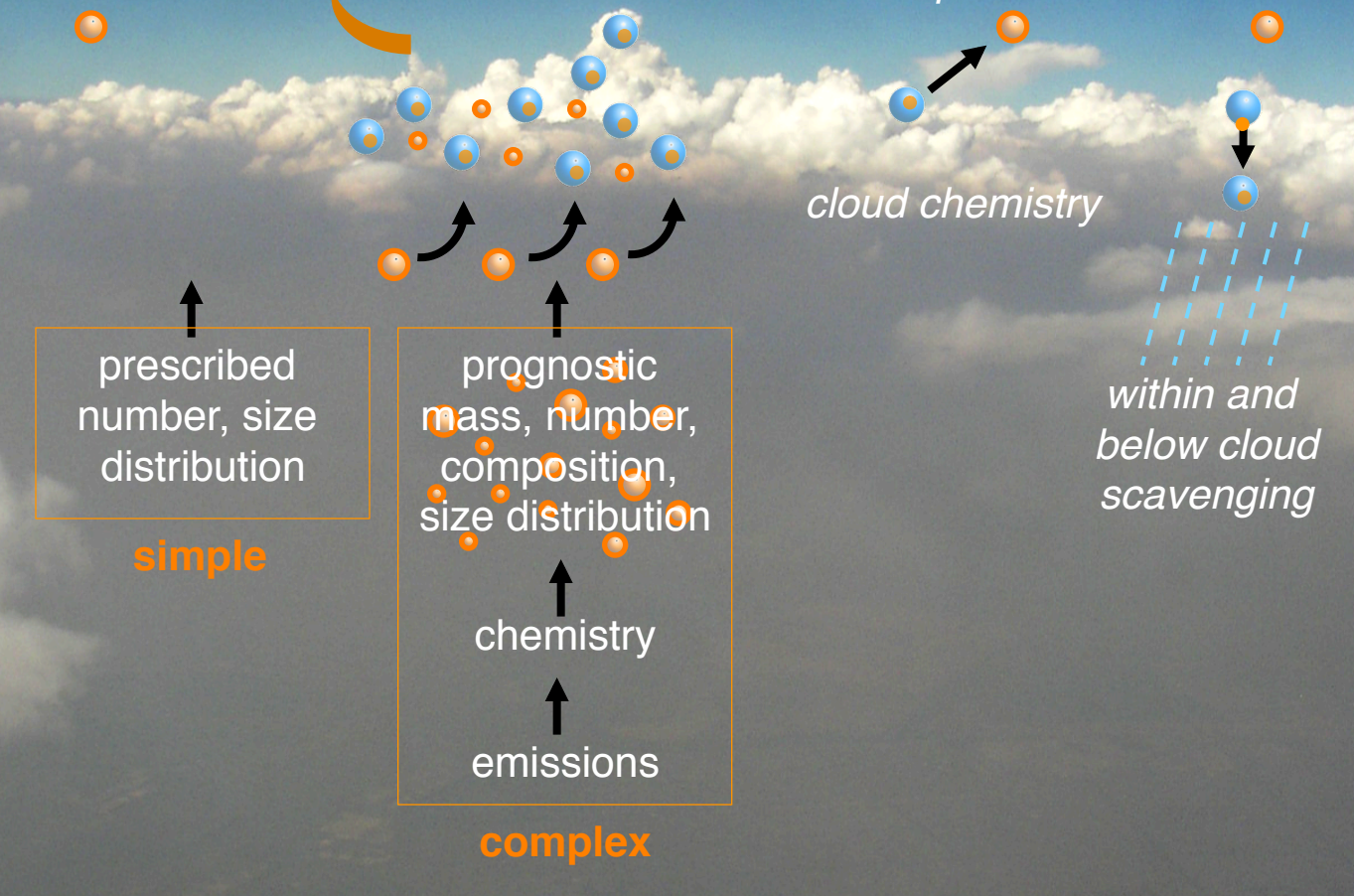
Cloud-Aerosol Interactions

General Description and Assumptions

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

Lin microphysics: includes cloud droplet # and modified autoconversion

interstitial → activation → cloud-borne → resuspension → interstitial



Simple:

- chem_opt = 0
- progn = 1
- naer = specified

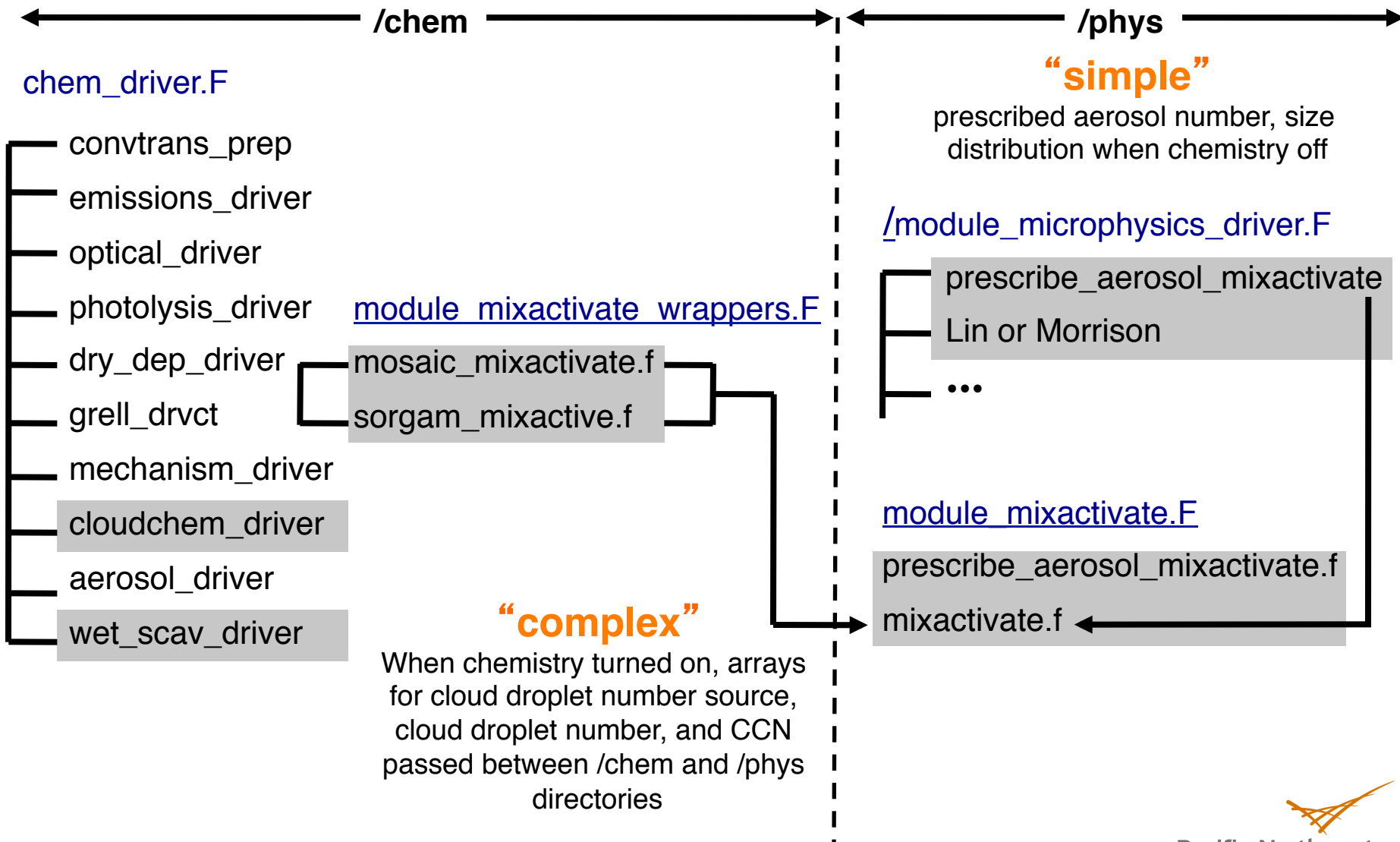
Complex:

- chem_opt = 9 – 12, 32, 34, 35
- progn=1
- naer = ignored

New for v3.3:

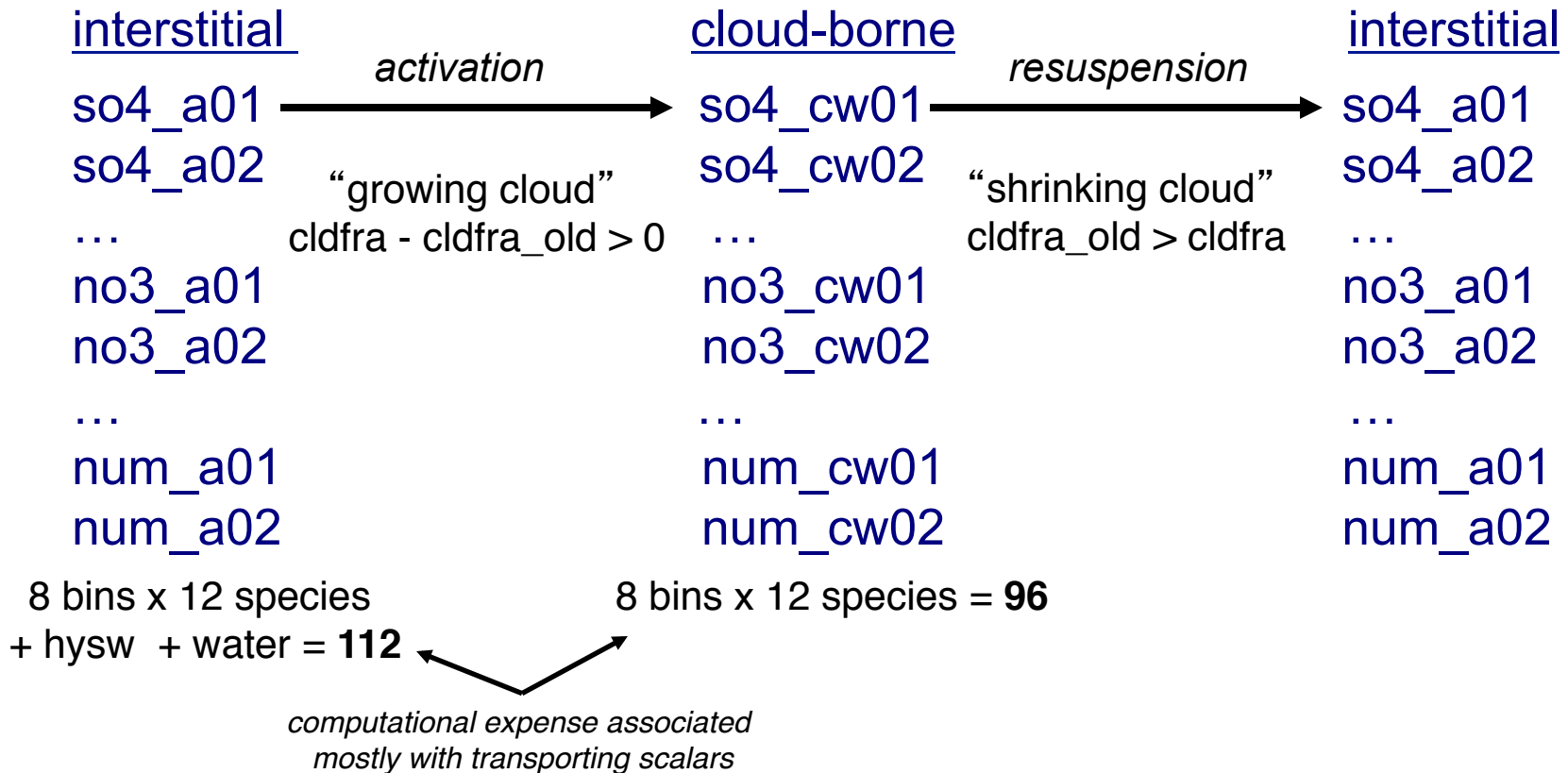
- Coupled to both Lin and Morrison microphysics

Flow Chart



Aerosol Species

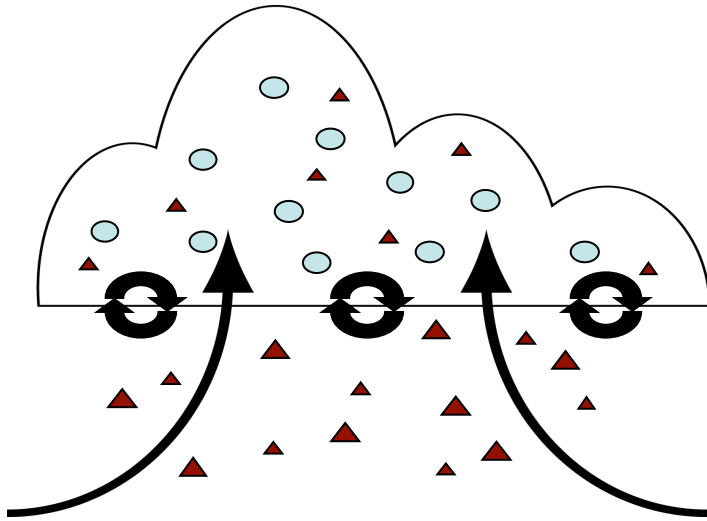
- interstitial and cloud-borne aerosol particles treated explicitly, nearly doubling the number of transported species



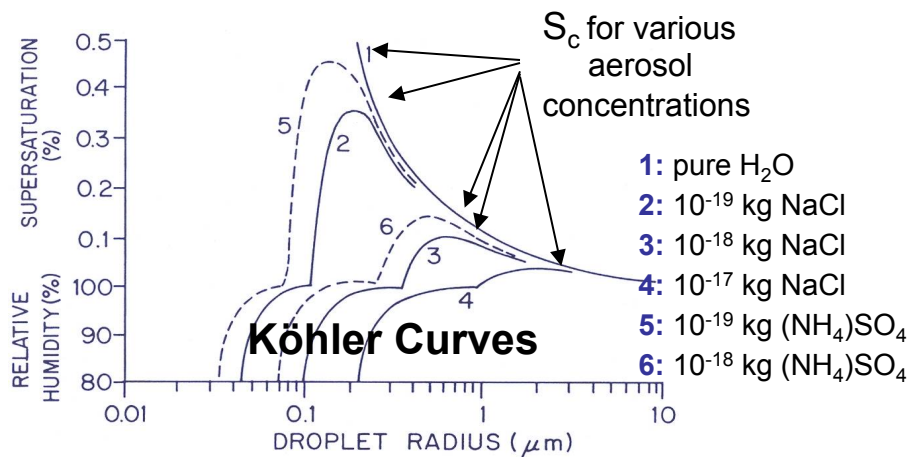
- similar for MADE/SORGAM: so4aj → so4cwj → so4aj



Activation



Aerosols activated when the environmental supersaturation in the air “entering cloud”, S_{\max} > aerosols critical supersaturation, S_c



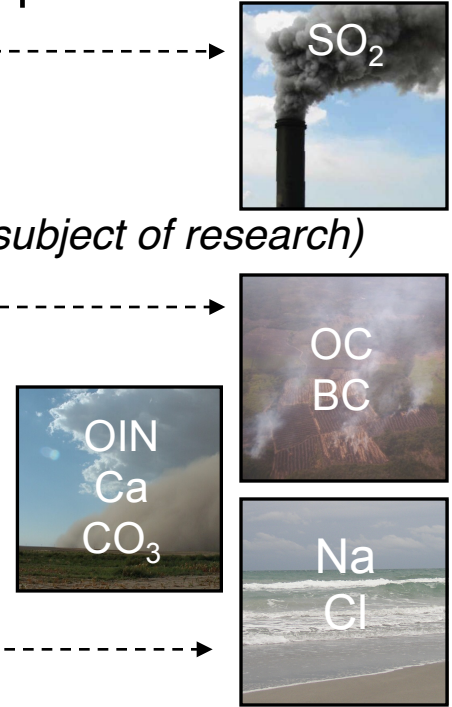
Activate.f computes activation fraction for mass and number for each bin/mode. Inputs include mean vertical velocity, $wbar$, and σ of the turbulent velocity spectrum, $sigw$.

Note: $sigw$ based on $exch_h$, but some PBL options (ACM) do not have $exch_h$ passed out of the subroutine. Minimum $exch_h$ set to 0.2 m s^{-1} since predicted values may be too low in free atmosphere.

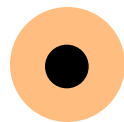
For each vertical velocity, peak S_{\max} depends on aerosol size and composition [Abdul Razzak and Ghan, 2000, 2002]. Activation fraction based distribution of S_c of the bin/mode - simply a fraction of aerosol mass or number in the bin/mode having $S_c < S_{\max}$

Hygroscopicity

- Hygroscopic properties depend on particulate composition:

- hygro_so4_aer = 0.5
 - hygro_no3_aer = 0.5
 - hygro_nh4_aer = 0.5
 - hygro_oc_aer = 0.14 (*some OC may be hygrophilic – subject of research*)
 - hygro_bc_aer = 1.0e-6 *hygrophobic*
 - hygro_oin_aer = 0.14
 - hygro_ca_aer = 0.1
 - hygro_co3_aer = 0.1
 - hygro_msa_aer = 0.58
 - hygro_cl_aer = 1.16 *hygrophilic*
 - hygro_na_aer = 1.16
- 

- Activation depends on **volume weighted bulk hygroscopicity**, prior to call to mixactivate.f in module_mixactivate_wrappers.F



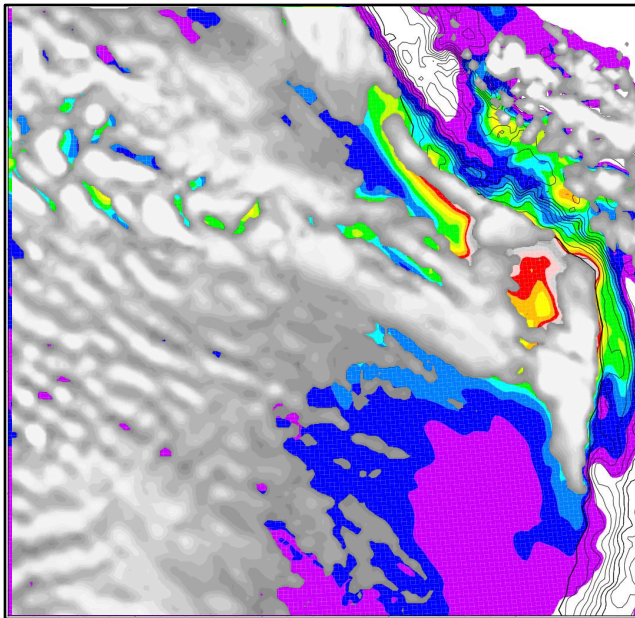
What about coating?

- For *chem_opt* = 0 and *nprog* = 1, hygroscopicity set to 0.5

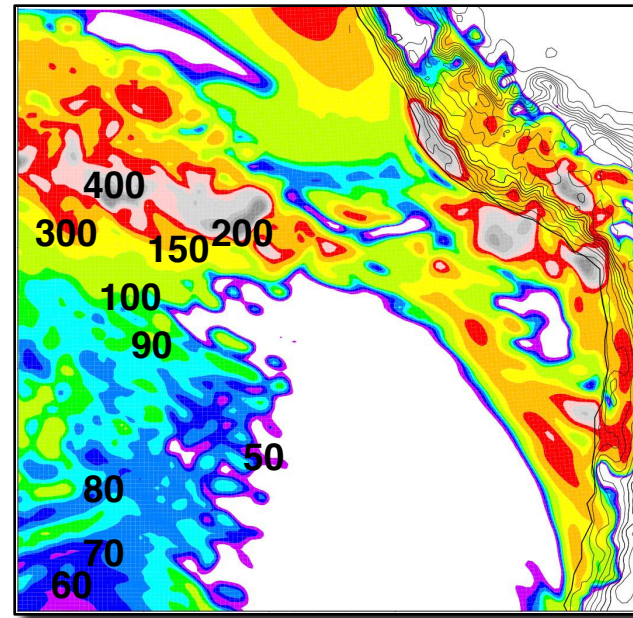
Cloud Condensation Nuclei

- CCN: number concentration of aerosols activated at a specified supersaturation → often have measured values to compare with
- Diagnostic quantity, varies in space and time
- Computed at 6 super-saturations (.02, .05, .1, .2, .5, and 1%) that correspond to *CCN1*, *CCN2*, *CCN3*, *CCN4*, *CCN5*, *CCN6* in Registry
- Computed in module_mixactivate.F

AOD (600 nm) and COD



CCN at 0.1% SS (# cm⁻³)



Cloud Droplet Number

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

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

qndrop →

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

qndropsourc

(nsource) →

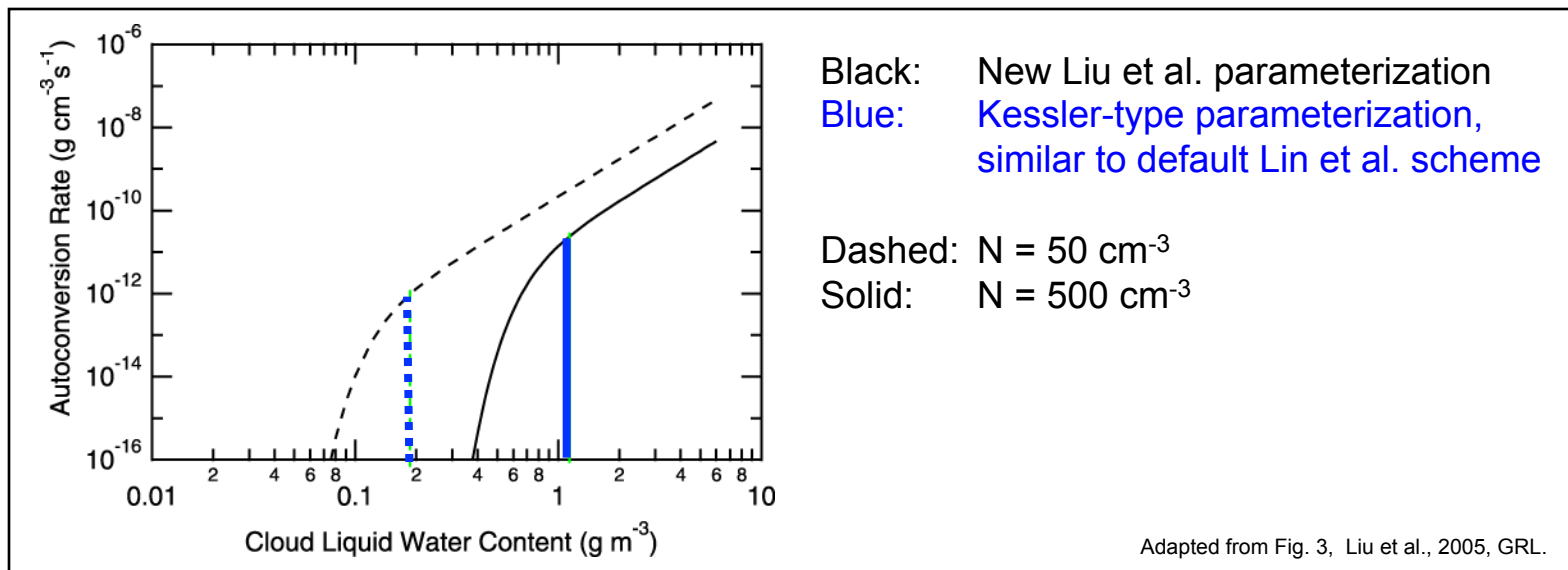
S_k - droplet source due to nucleation (determined in mixactivate.f)

- 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 the cloud optical depth in Goddard or RRTMG shortwave radiation scheme (*ra_sw_physics* = 2 or 4)



Autoconversion

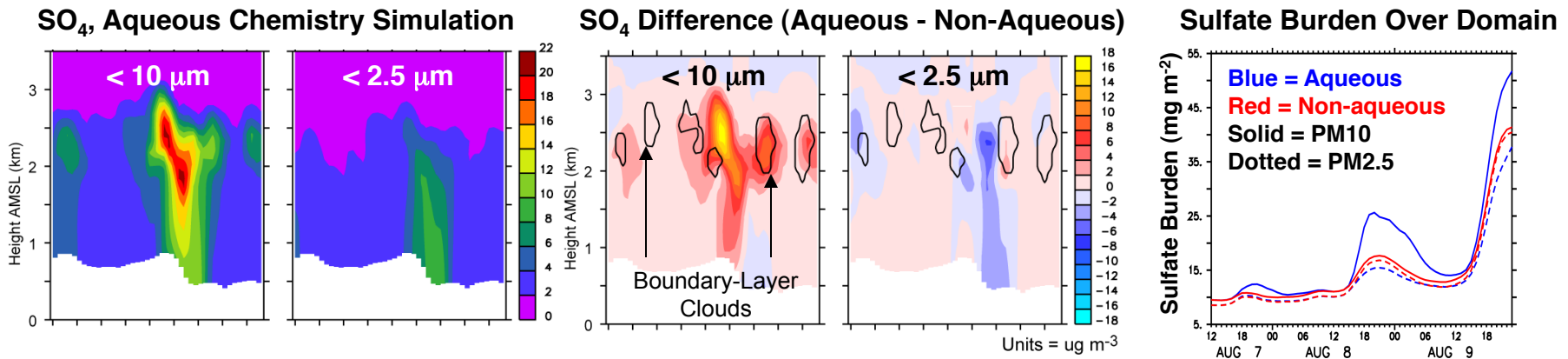
- autoconversion = coalescence of cloud droplets to form embryonic rain drops
- replaced autoconversion parameterization employed by Lin et al. microphysics ($mp_physics = 2$) with *Liu et al. [2005]* parameterization
 - adds droplet number dependence
 - physically based w/o tunable parameters



Aqueous Chemistry

- Bulk cloud-chemistry module of *Fahey and Pandis* [2001] compatible with MOSAIC and MADE/SORGAM (cloudchem_driver.F)
- Chemistry in cloud drops, but not rain drops
- Oxidation of S(IV) by H_2O_2 , O_3 , trace metals, and radical species, as well as 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; assumptions regarding the cloud water fraction for each bin/mode

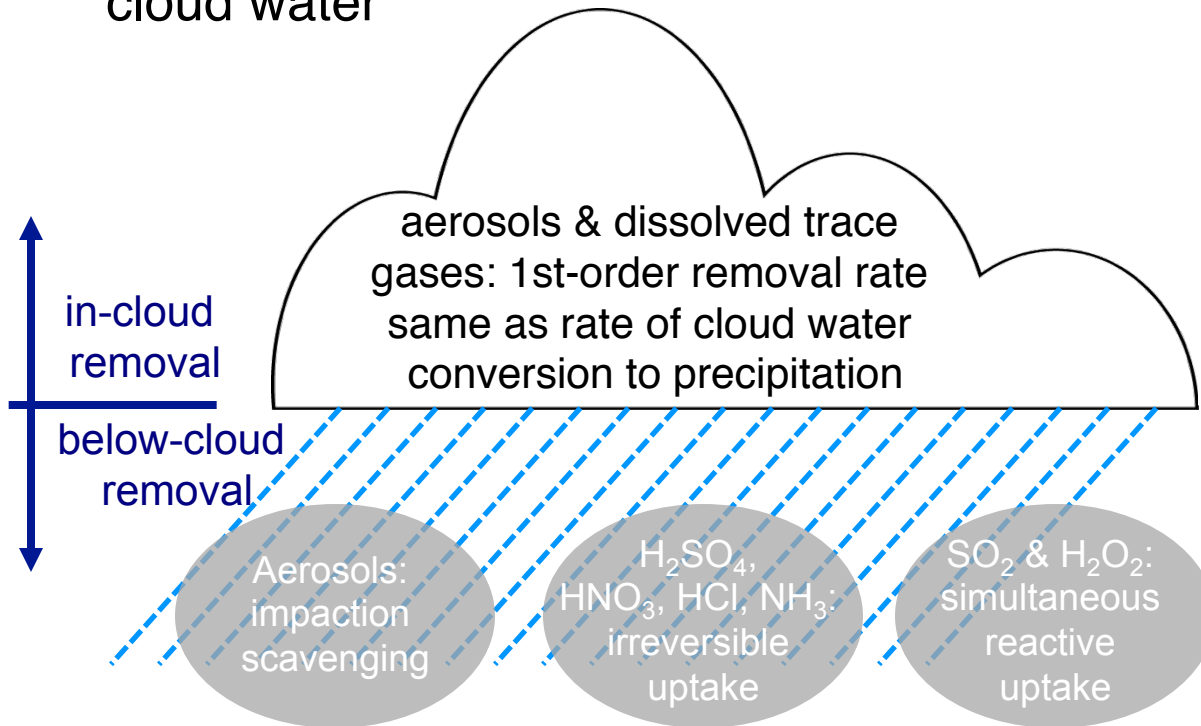
Vertical Cross-Section Through Power Plant SO_2 Plume



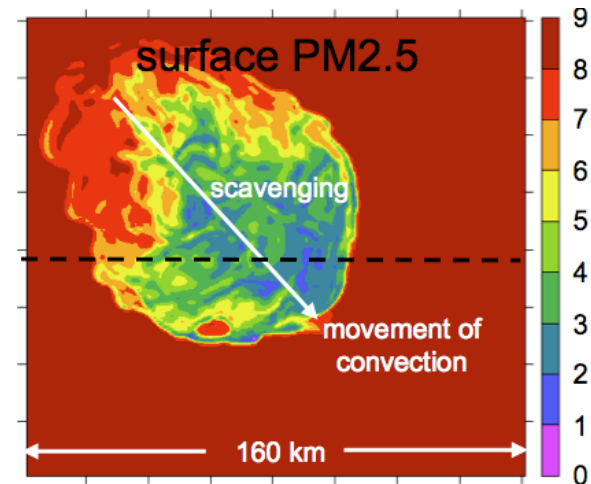
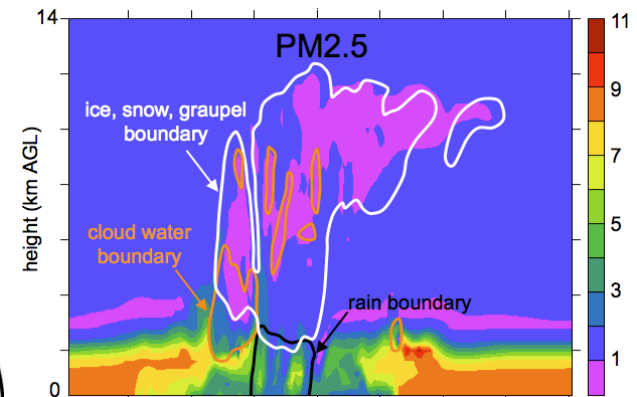
- Aqueous chemistry in module_ctrans_greldrct.F being developed (MADE/SORGAM only)

Wet Removal - Scavenging

- As cloud drops are collected by precipitation particles (rain, snow, graupel), cloud-borne aerosols and trace gases are also collected
- While cloud-borne aerosols are explicit, the cloud chemistry module provides the fraction of trace gas that is cloud-borne or dissolved in cloud water

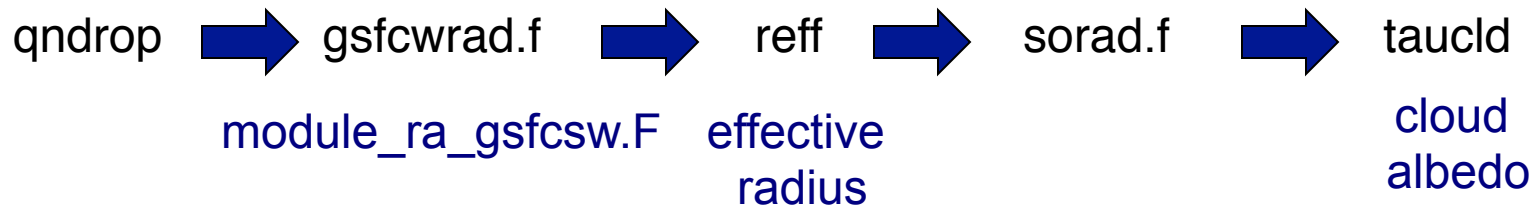
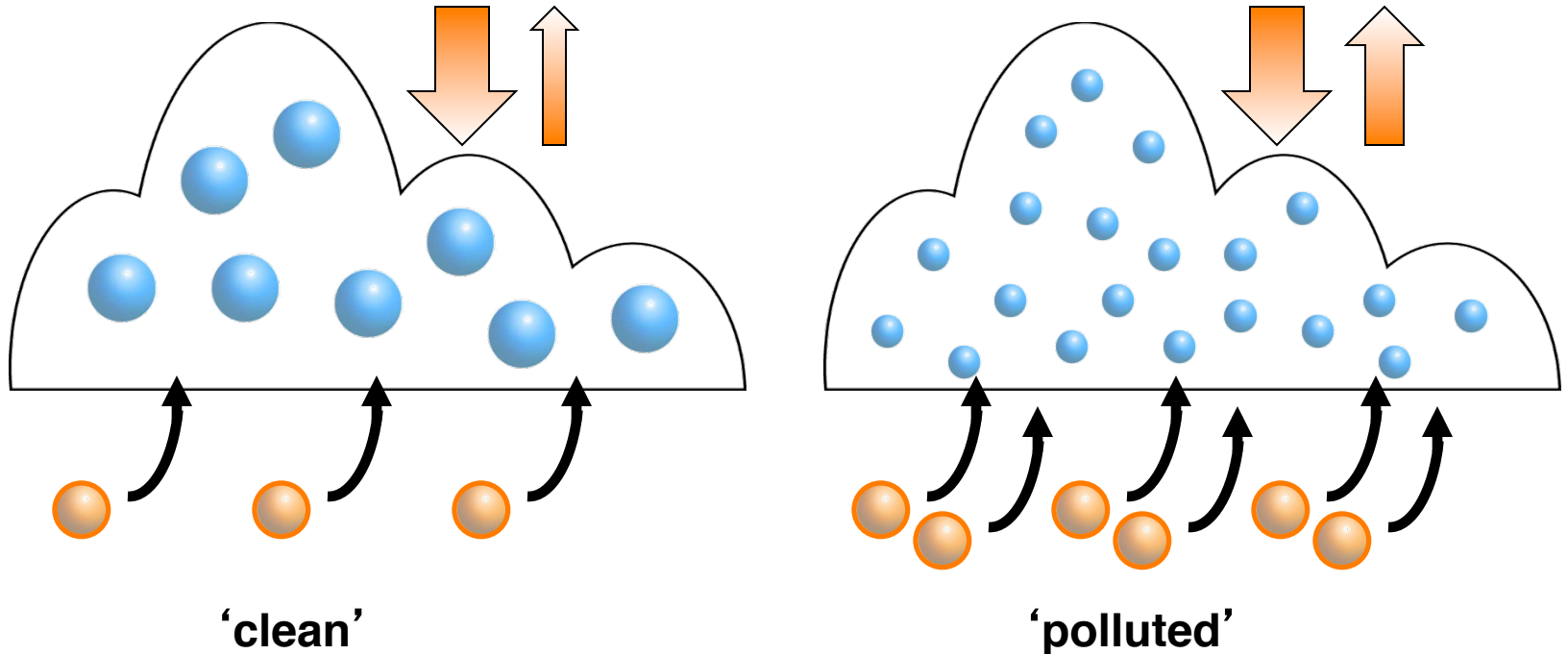


scavenged aerosols and gases instantly removed (but not saved) see *Easter et al.* [2004], also aerosols are not resuspended for evaporating rain



First Indirect Effect

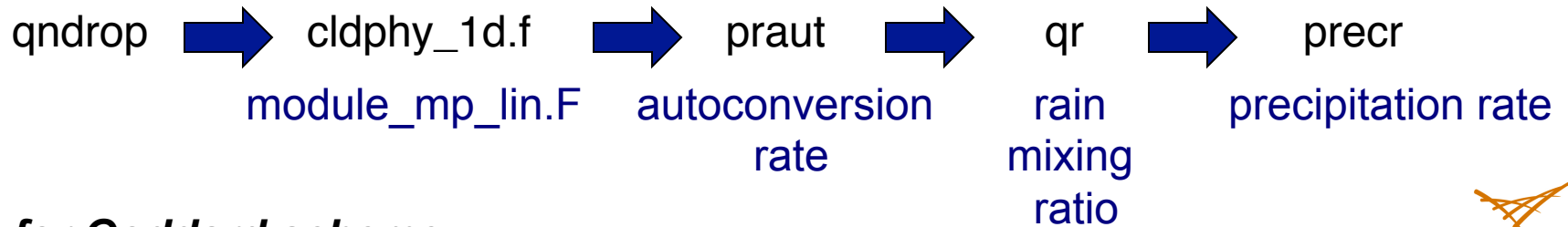
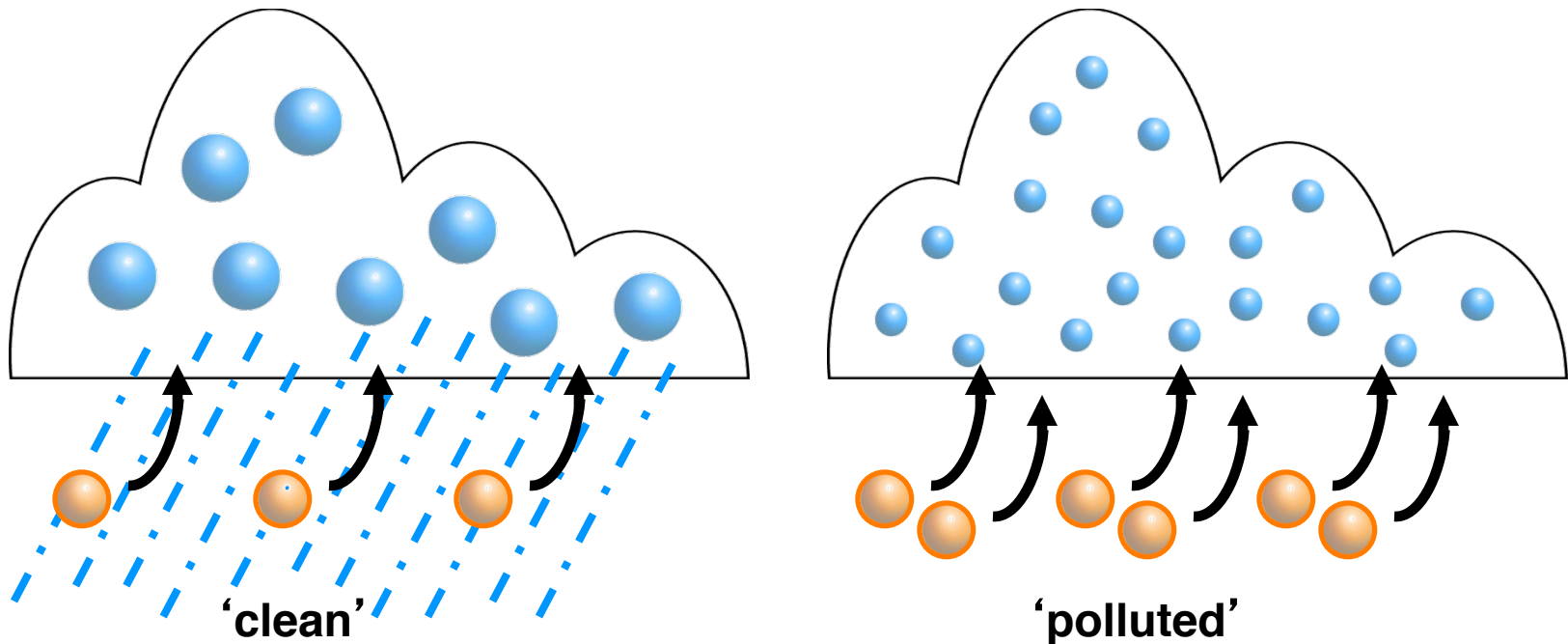
- Influence of cloud optical depth through impact on effective radius, with no change in water content of cloud



for Goddard scheme

Second Indirect Effect

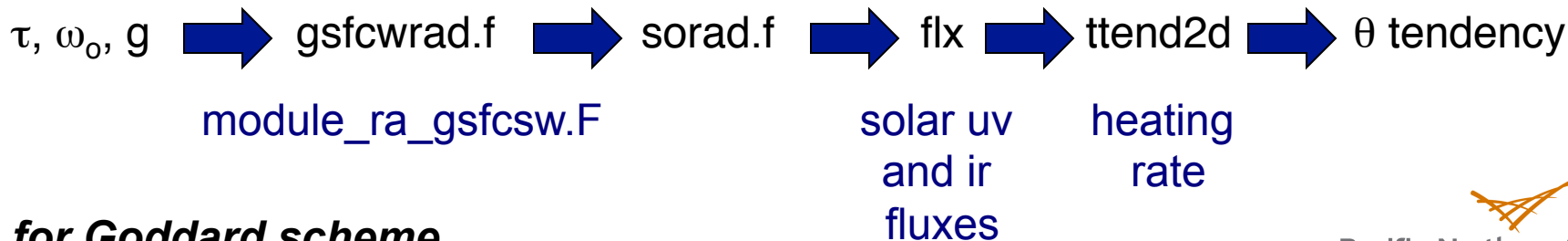
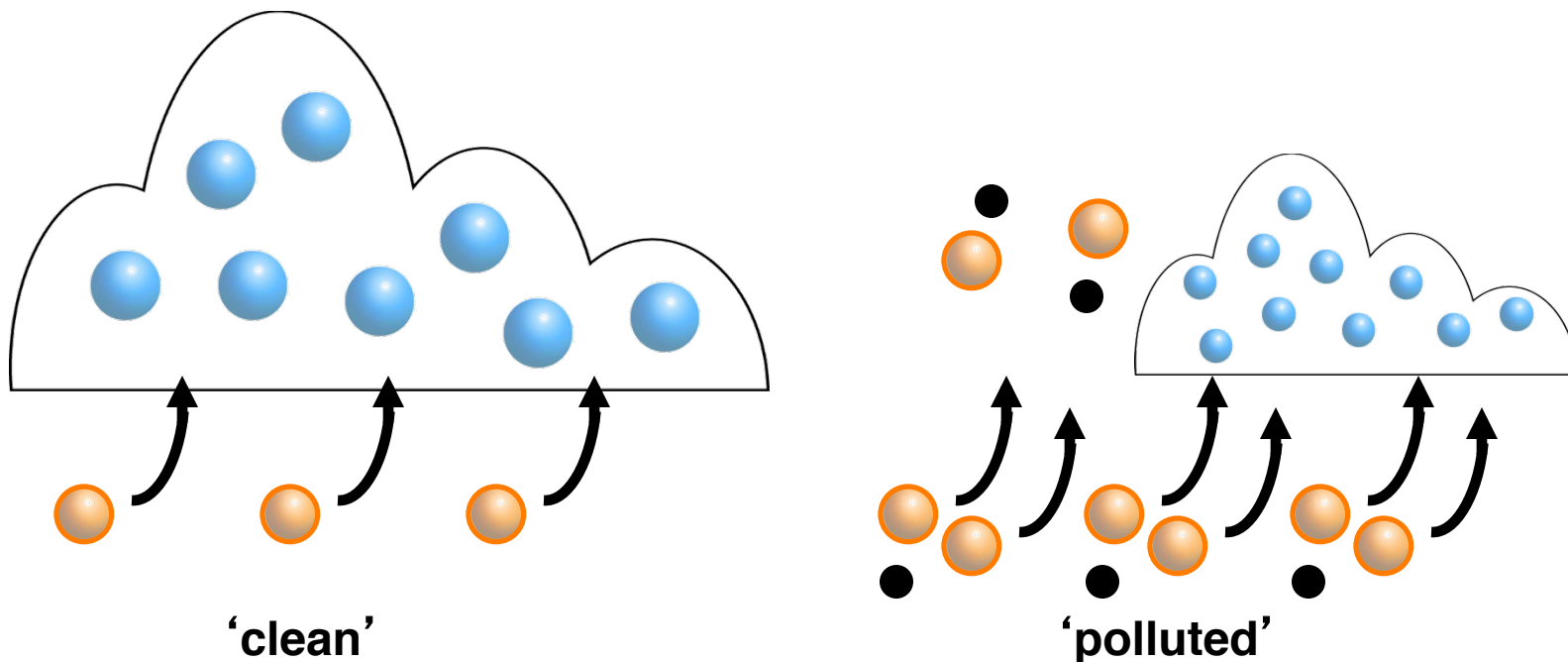
- Influence of cloud optical depth through influence of droplet number on mean droplet size and hence initiation of precipitation



for Goddard scheme

Semi-Direct Effect

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



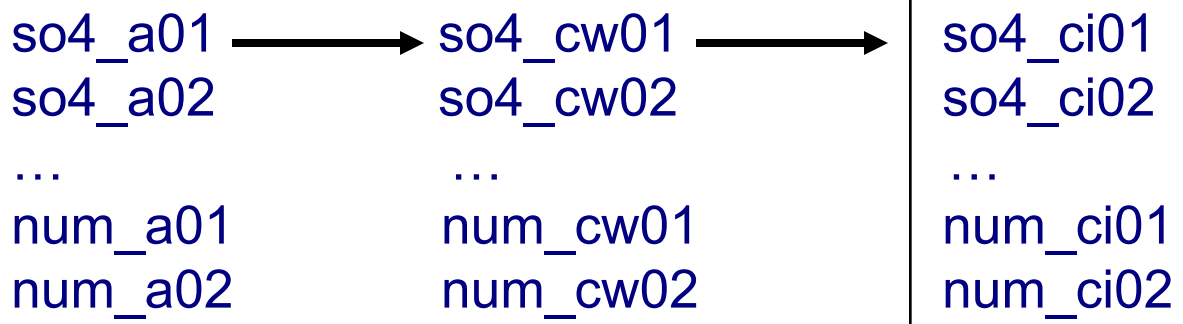
for Goddard scheme

Interactions not Treated

- **First Dispersion Effect:** Affects cloud optical depth via the influence of aerosols on the width of the droplet size distribution, with no change in water content of cloud
- **Second Dispersion Effect:** Affects cloud optical depth via the influence of aerosols on the width of the droplet size distribution 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

(Ice processes are a current research topic for PNNL, NCAR, others)

pointer system already in place to handle ice-borne species



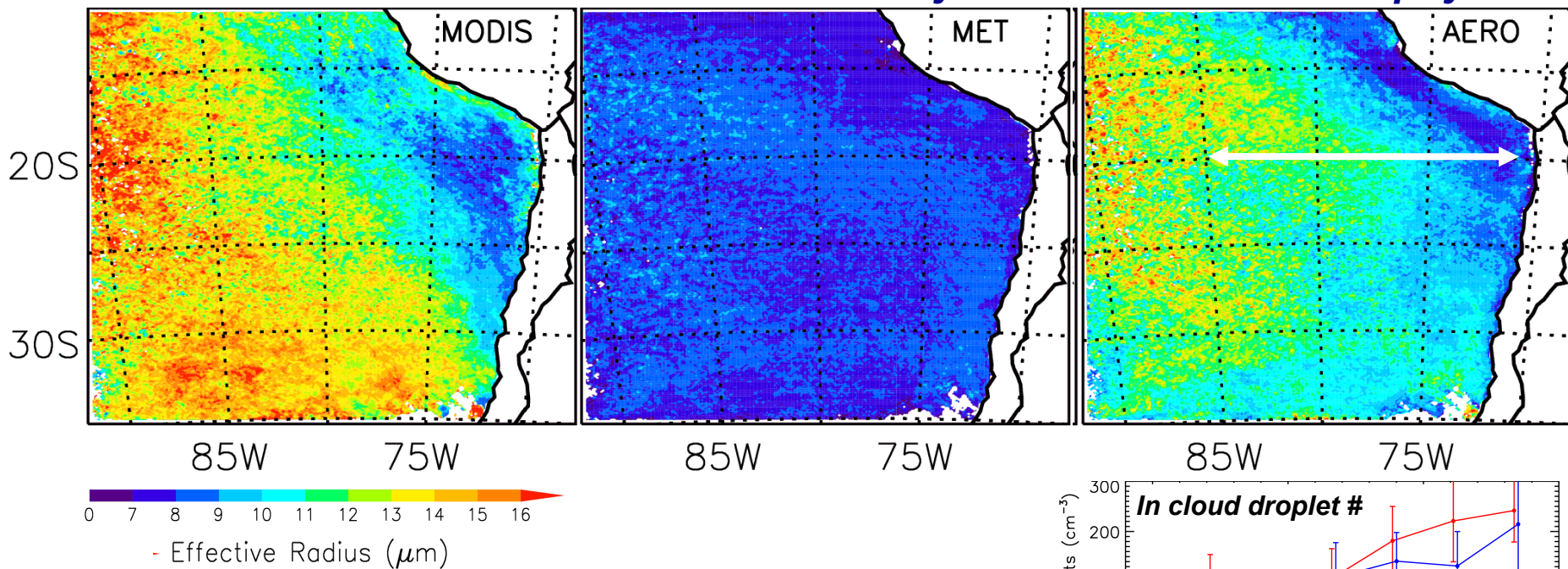
Example 1: Marine Stratocumulus

Average Effective Droplet Radius during 2008 VOCALS-REx

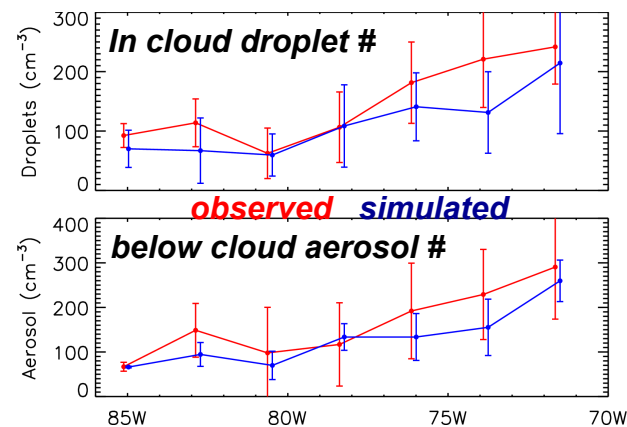
MODIS

**WRF
no chemistry**

**MOSAIC aerosols and
Morrison microphysics**



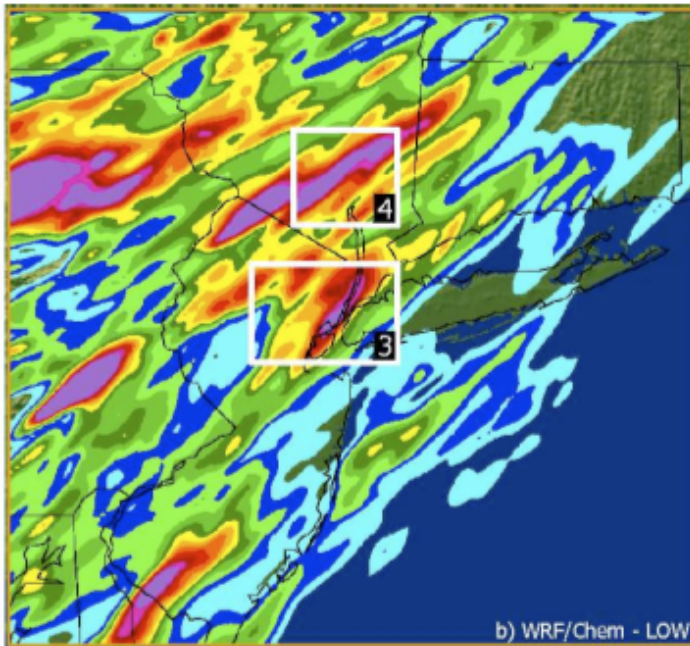
- Yang, Q. W.I. Gustafson Jr., J.D. Fast, H. Wang, R.C. Easter, and H. Morrison, 2011: Assessing regional scale predictions of aerosols, marine stratocumulus, and their interactions during VOCALS-REx using WRF-Chem. To appear in *Atmos. Chem. Phys. Discuss.*



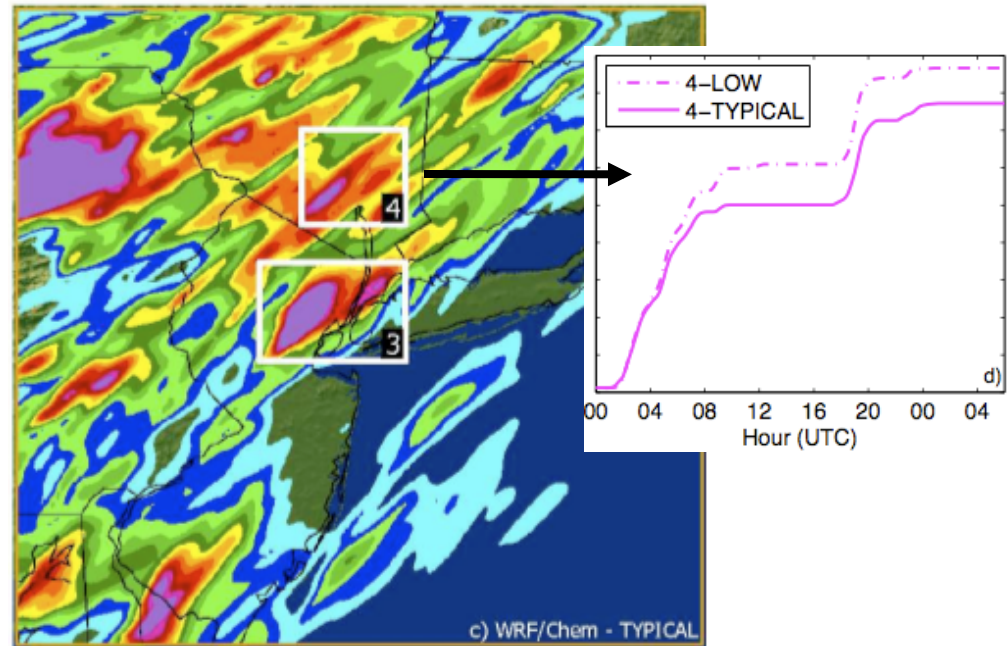
Example 2: *Deep Convection and Urban Aerosols*

Impact of Particulates on Convective Precipitation Along the Urban East Coast Corridor

WRF-Chem: low emissions



WRF-Chem: typical emissions



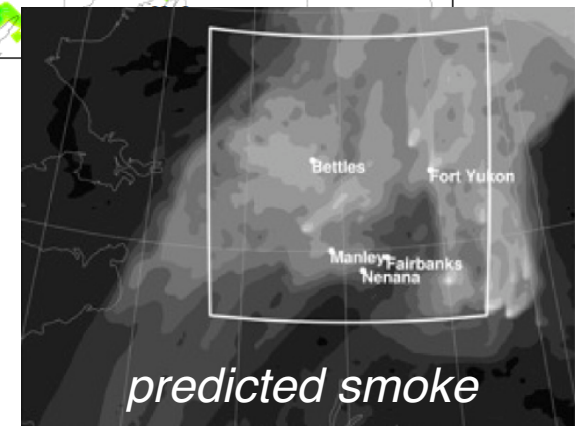
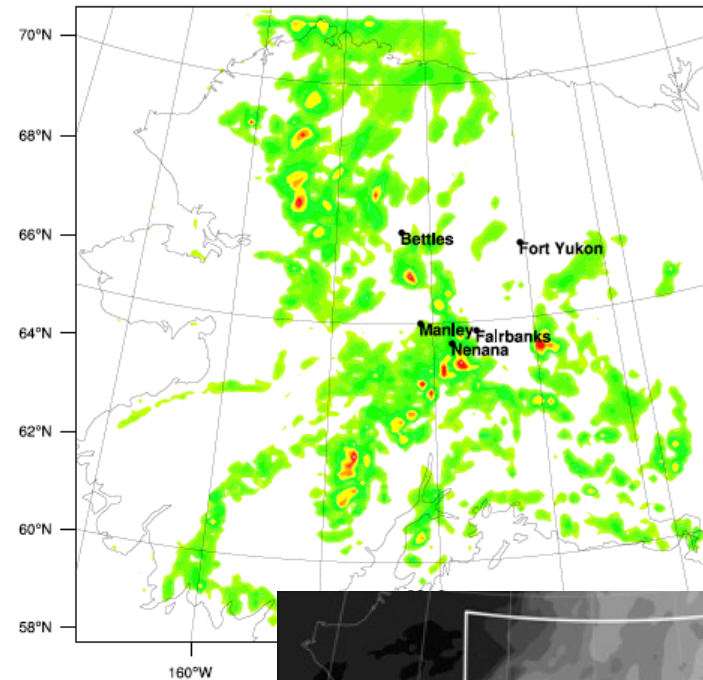
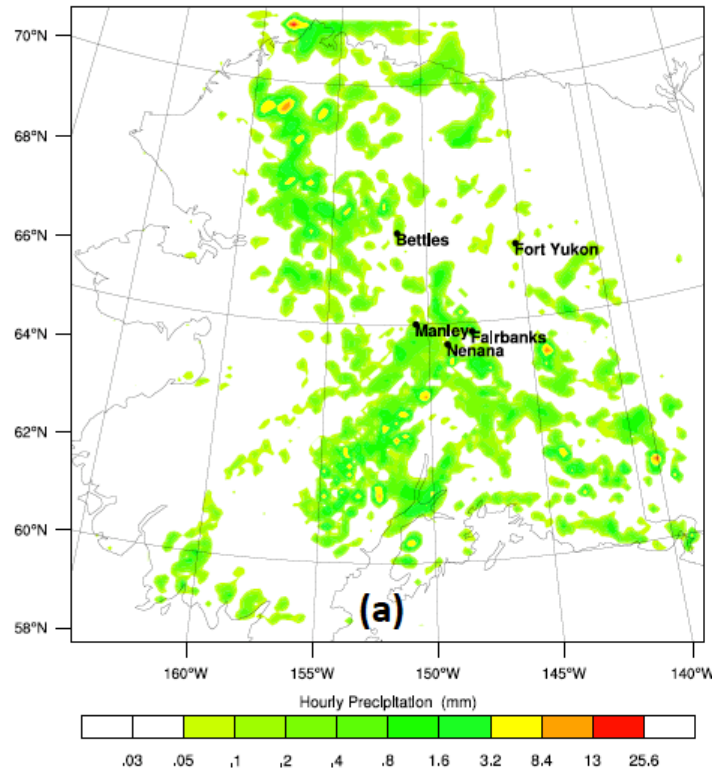
- Ntelekos, A., J.A. Smith, L. Donner, J.D. Fast, E.G. Chapman, W.I. Gustafson Jr., and W.F. Krajewski, 2008: The Effects of aerosols on intense convective precipitation in the northeastern U.S. *Q. J. Roy. Meteor. Soc.*, 135, 1367-1391.

Example 3: *Smoke Entrained into Clouds*

Precipitation over Alaska

Without aerosol-cloud interactions

With aerosol-cloud interactions



- Grell, G.A., S.R. Frietas, M. Stuefer, and J.D. Fast, 2008: Inclusion of biomass burning in WRF-Chem: Impact of wildfires on weather forecasts. *Atmos. Chem. Phys.*, 11, 5229-5303.

Settings in namelist.input

Simple:

- *chem_opt* = 0
- *naer* = specified value

Complex:

- *chem_opt* = 9 - 12, 32, 34, 35 - cloud-phase aerosols for MOSAIC and MADE/SORGAM
- *cldchem_onoff* = 1, turns on cloud chemistry
- *wetscav_onoff* = 1, turns on wet scavenging

Both:

- *mp_physics* = 2, 10 - cloud-aerosol interactions only Lin and Morrison schemes only
- *progn* = 1, turns on prognostic cloud droplet number



Comparing Options

Care Must be Taken in Quantifying Direct and Indirect Effects!

- **Direct Effect:**

- Run with *aer_ra_feedback* on versus off, or
- Add code to output clean-sky and dirty-sky from the same run

- **Indirect Effects:**

- Comparing a *chem_opt* = 8 with a *chem_opt* = 10 for MOSAIC run **does not** quantify the indirect effect since the autoconversion scheme used in the Lin microphysics scheme will be different
- Need to determine a prescribed aerosol scenario to compare with *chem_opt* = 10 – see *Gustafson et al.*, GRL, [2007]
- An approach used with GCMs is to output dirty-cloudy, dirty-clear, clean-cloudy, and clean-cloudy radiation from the same run

- **Indirect Effects Usage:**

- Works with microphysics only – not cumulus parameterizations
- There are proposed efforts to extend cloud-aerosol interactions to cumulus parameterizations (for $\Delta x > 10$ km); need to worry about double counting
- In addition to *Abdul-Razaak and Ghan* [2000, 2002], other schemes have been used to compute aerosol activation [*Foutoukis and Nenes*, 2005]



Future Capabilities

Coming Soon (under development):

- Parameterization from CAM5 global climate model ported to WRF to represent effect of aerosols on **ice-phase clouds** via ice nucleation (IN)
- Aerosol-cloud interactions coupled with **cumulus parameterizations** for simulations $\Delta x > 10$ km
- **Separate wet removal scheme** not coupled with aerosol indirect effect
- Studies at PNNL underway include those for CHAPS (shallow fair-weather cumulus), ISDAC/ARCTAS (mixed-phase clouds), and additional papers on VOCALS (marine stratocumulus)
- NCAR scientists working on aerosols and chemistry in deep convective clouds
- Others by WRF-Chem users ...

For more information and updates:

- PNNL modules: www.pnl.gov/atmospheric/research/wrf-chem
- See web page for list of papers on aerosol-cloud interactions

Aerosol Modeling Testbed

- Better **quantify uncertainties** by targeting specific processes
- Provide tools to **facilitate science** by minimizing redundant tasks
- **Document** performance and computational expense
- Build **internationally-recognized capability** that fosters collaboration

Published in March
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THE AEROSOL MODELING TESTBED A Community Tool to Objectively Evaluate Aerosol Process Modules

BY JEROME D. FAST, WILLIAM I. GUSTAFSON JR., ELAINE C. CHARMAN, RICHARD C. EASTER,
JIMMY P. BISHOP, RAJAN A. ZAWAR, GEORGE A. O'NEILL, AND MARY C. BATH

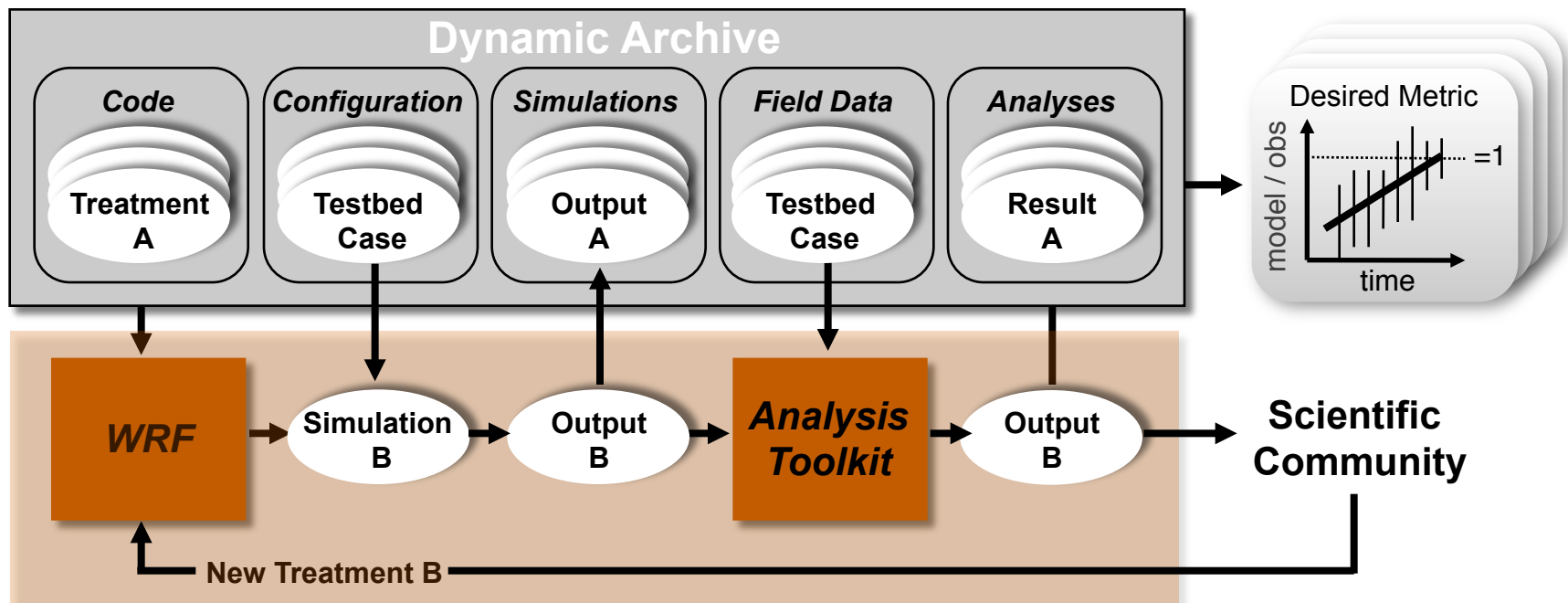
The test bed is a new computational framework to streamline the process of testing and evaluating aerosol process modules over a range of spatial and temporal scales.

Many of the uncertainties associated with estimates of direct (via scattering and absorption of radiation by aerosols) and indirect (via droplet nucleation influenced by aerosols) radiative forcing in climate models (Gordon et al. 2007) can be attributed to inaccurate simulations of the spatial and temporal variations of aerosol mass, number, composition, mixing state, size distribution, hygroscopicity, and optical properties. For example, the formation and transformation of secondary organic aerosols (SOAs, e.g., Volkamer et al. 2006) and the nature of many cloud-aerosol interactions (e.g., Lohmann and Feichter 2005) are still poorly understood and consequently inadequately represented in models. The coarse horizontal and vertical grid spacings usually employed by global climate models, which cannot resolve the observed spatial variability of atmospheric aerosols as well as meteorological factors that contribute to aerosol-radiation-cloud-chemistry interactions (e.g., Haywood et al. 1997; Petz 2001), are another factor that contributes to uncertainties in predictions of aerosol radiative forcing.

Regional and global models are becoming more complex as they incorporate new representations for the size distribution of aerosol mass and number and new parameterizations of aerosol processes. Journal articles that describe new parameterizations of aerosol processes usually employ a single model along with a dataset for a specific region and/or time period to quantify the performance of the new parameterization. The models, evaluation datasets, and other factors differ from study to study. One consequence of the current modeling paradigm is that the performance and computational efficiency of multiple treatments for a specific aerosol process cannot be quantitatively compared, because many other processes among aerosol models are different

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Community Tools

‘Analysis Toolkit’ – Analogous to MET Software

Extraction Programs – “Simulators”

extracts model variables compatible with a wide range of observation types



Analysis Programs

produces *graphics* and *statistics* that examines model performance

Largely automatic – scripts do everything by default, but customizable

Designed to evolve in time:

- PNNL will be developing additional capabilities
- Users can contribute to capabilities