Aerosol-Radiation-Microphysics Interactions

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NCAR

But content by

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WRF-Chem Tutorial, February 7, 2017, Boulder CO

Motivation

Use WRF-Chem to study local to regional-scale evolution of particulates and their effect on radiation, clouds, and chemistry

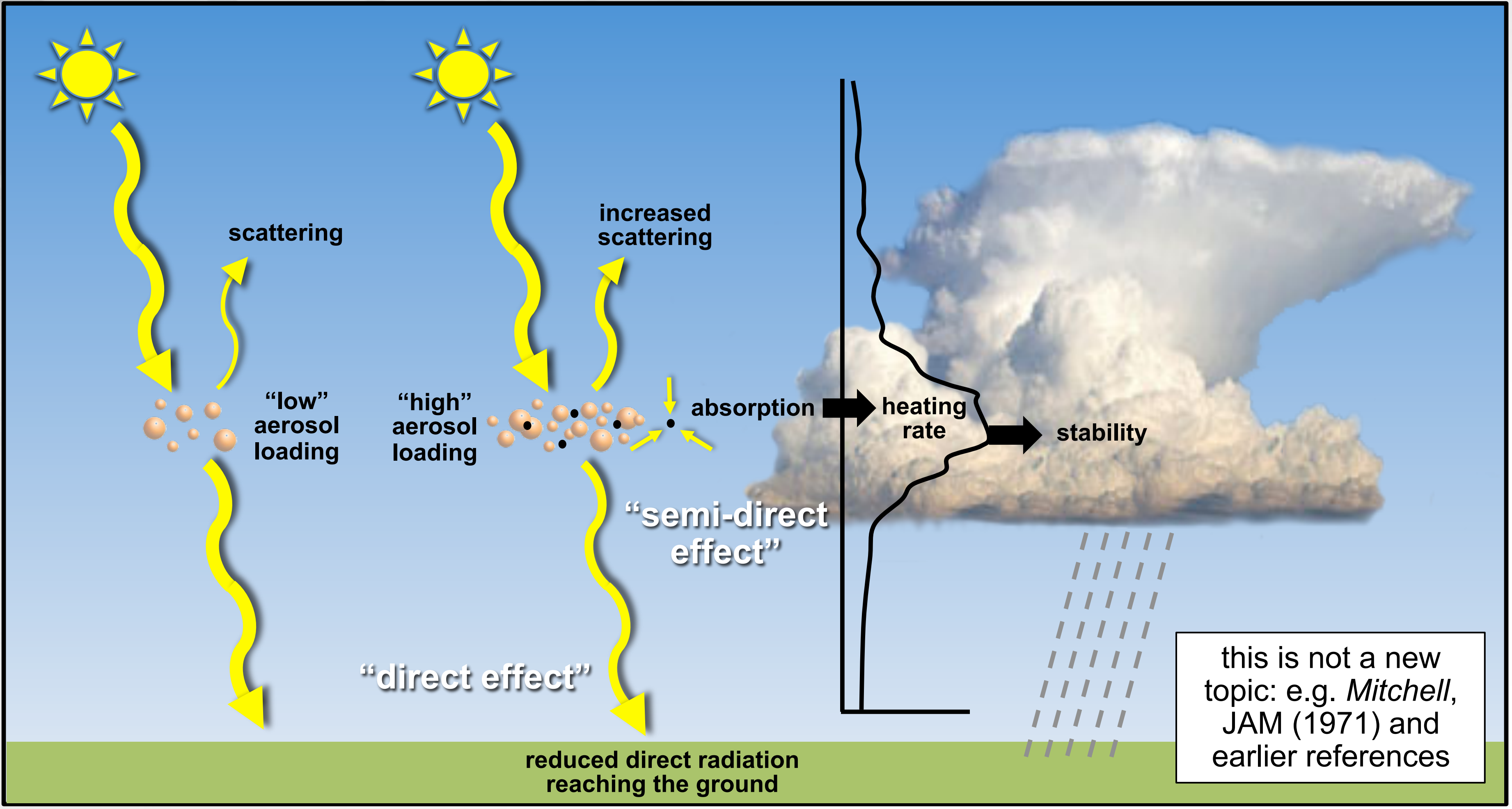
A Brief History …

- First, aerosol-radiation-cloud interactions were coupled to the MOSAIC aerosol model, adapted from those used in a global climate model
- Aerosol-radiation-cloud interactions have been expanded to handle more aerosol models (GOCART, MADE/SORGAM, MAM) and microphysics schemes (Lin, Morrison, Morrison-Gettelman)
- More capabilities are being added and tested, making modules more generic, and trying to follow WRF coding guidelines

Outline:

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

Part 1: Aerosol Direct Effects



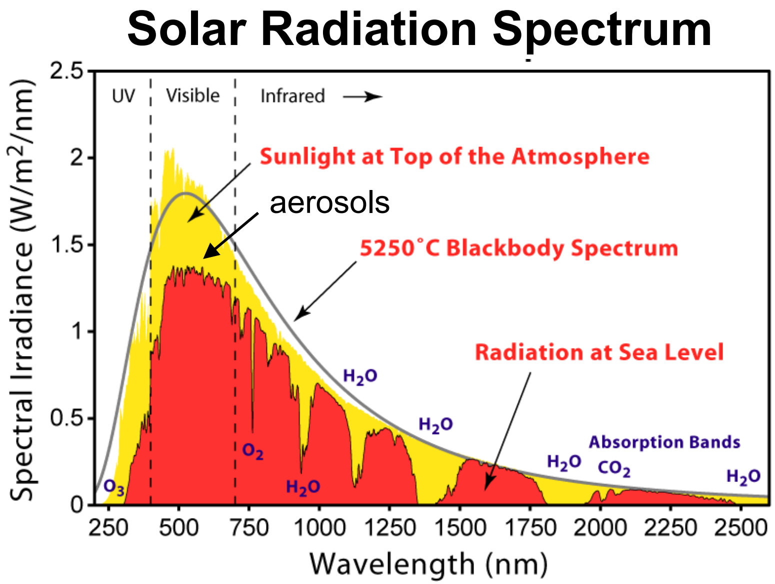
this is not a new topic: e.g. *Mitchell*, JAM (1971) and earlier references

In additions to water vapor, carbon dioxide, ozone, and other trace gases, aerosols can also affect the radiation budget, and atmospheric stability

surface heat and latent heat fluxes → **boundary layer temperature and moisture** → **clouds**

Aerosols in Relation to Radiation Modules

- Aerosols affect radiation mostly in the visible wavelength region
- In contrast with water vapor, carbon dioxide, and ozone, the temporal and spatial variability of aerosols is much larger and difficult to simulate
  - **Episodic Sources:** dust, biomass burning, volcanic (potentially large concentrations)
  - **More "Continuous" Sources:** sea-salt, biogenic, anthropogenic (usually smaller concentrations)



How are aerosol effects accounted for in atmospheric models?

- **Ignored** - no effect of aerosols on radiation
- Use prescribed or **climatological** aerosol properties – that may vary in space and seasonally (not discussed in this presentation)
- Use **prognostic aerosols** (e.g. WRF-Chem)

Aerosol Optical Properties:
Aerosol Optical Depth (AOD)

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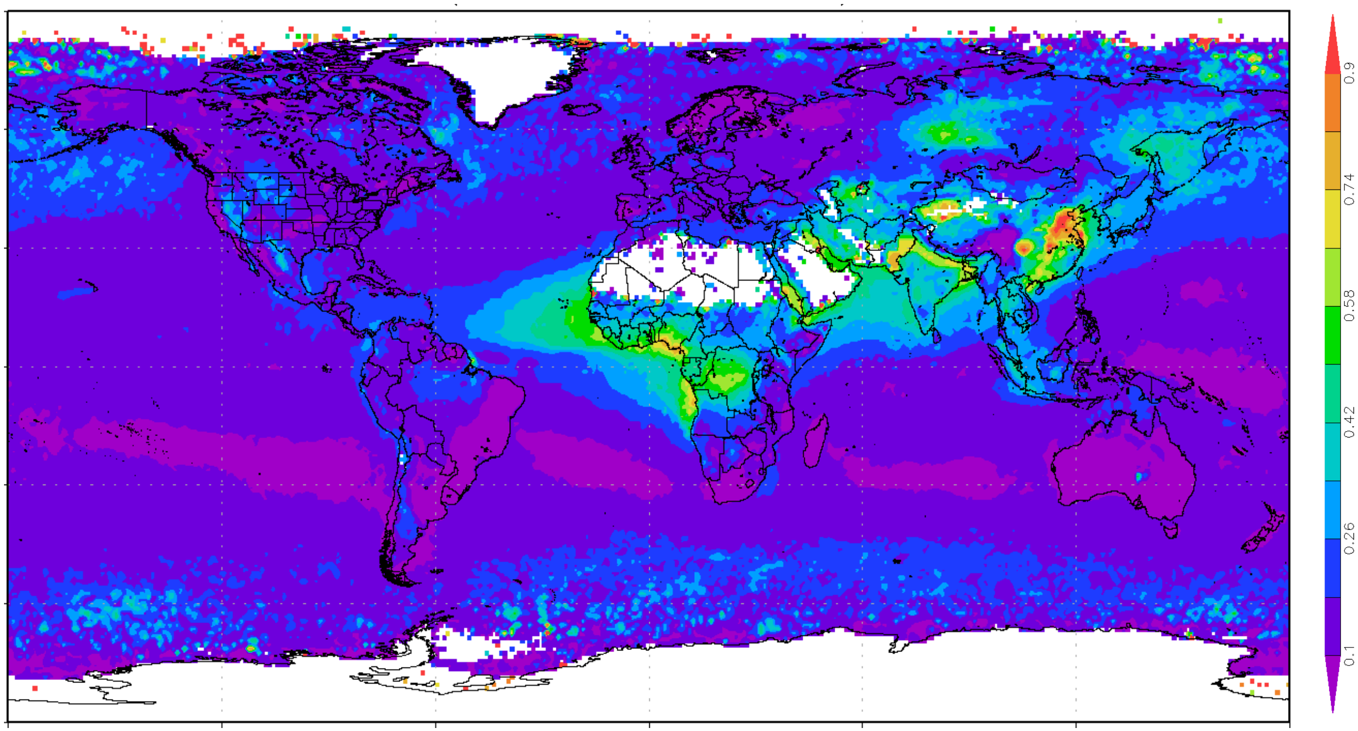
- **Extinction coefficient**: fractional depletion of radiance per unit path length (km^{-1}) due to scattering and absorption by aerosols
- **Aerosol optical depth** (AOD) or **thickness** (AOT): integrated extinction coefficient over a vertical column, $I / I_o = e^{-AOD}$
  - AOD = 0 no aerosol effect
  - AOD ~ 1 "large"
  - AOD > 1 extremely high aerosol concentrations



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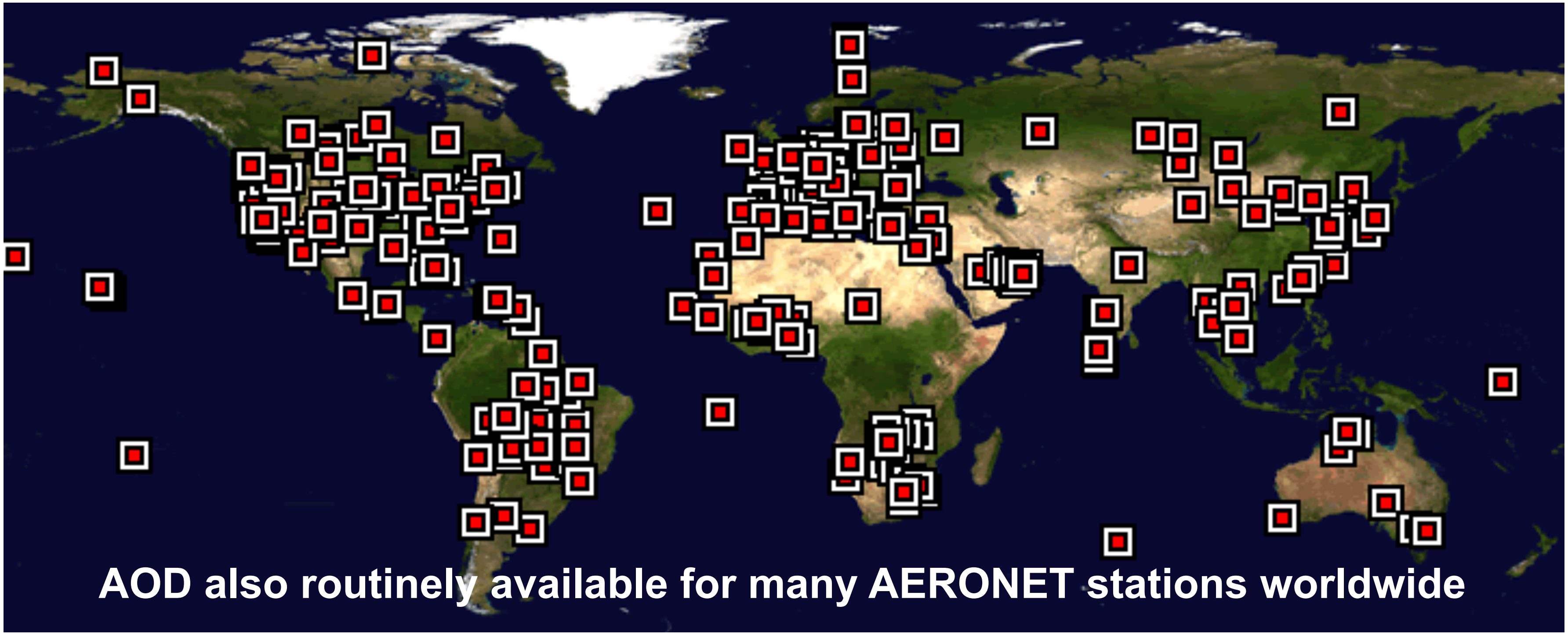
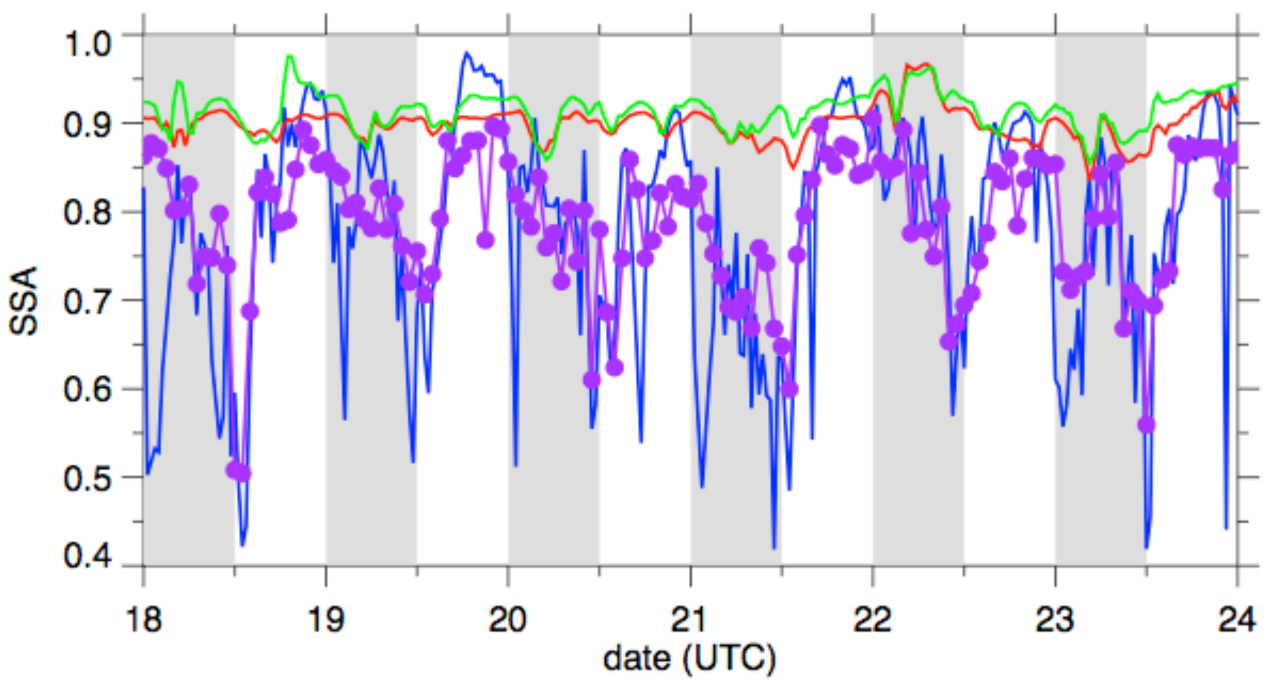


AOD also routinely available for many AERONET stations worldwide

Aerosol Optical Properties:
Single Scattering Albedo, w_o

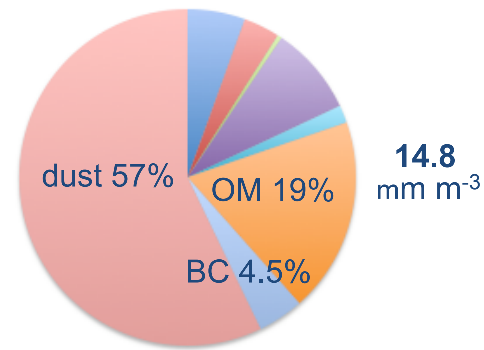
- SSA is ratio of scattering to extinction efficiency, $w_o = k_s / (k_a+k_s)$
  can be measured
  - SSA = 1 all particle extinction due to scattering
  - SSA = 0 all particle extinction due to absorption (does not happen in reality)
- Models simulate AOD_l “reasonably well”, but there are large uncertainties in w_o

SSA_{870nm} near Mexico City

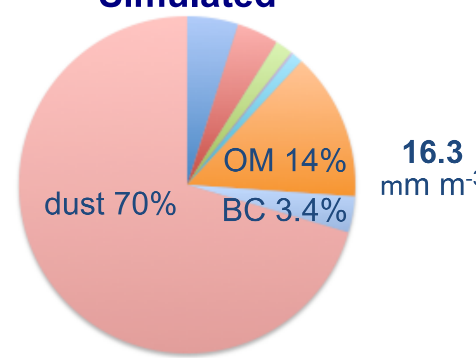


aerosol optical properties driven by measurements

Observed 12 UTC March 20

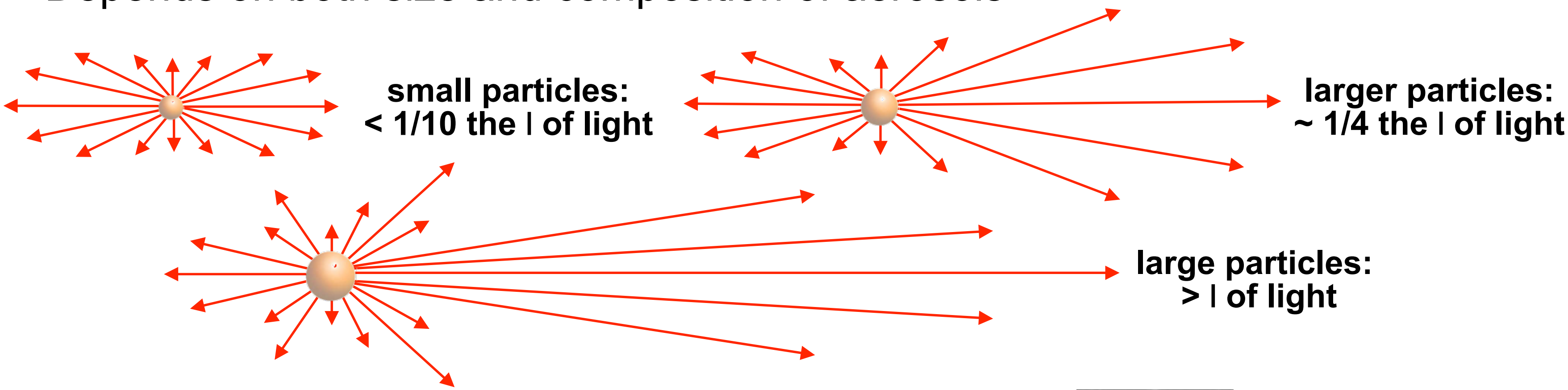


Simulated



Aerosol Optical Properties:
Asymmetry Factor, g

- Preferred scattering direction (forward or backward) for the light encountering the aerosol particles
  - Approaches 1 for scattering strongly peaked in the forward direction
  - Approaches -1 for scattering strongly peaked in the backward direction
  - g = 0 means scattering evenly distributed between forward and backward scattering (isotropic scattering – such as from small particles)
- Depends on both size and composition of aerosols



- Theoretical relationships used to derive g from measurements

Methodology for Prognostic Aerosols

Generic Aerosol Optical Property Module

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

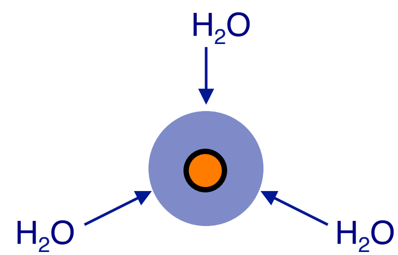
- AOD, ω_o, and g computed at
  4 wavelengths (**300, 400, 600, 1000** nm) for shortwave radiation
  16 wavelengths for longwave radiation

Angstrom exponent used to convert to wavelengths needed by radiation schemes

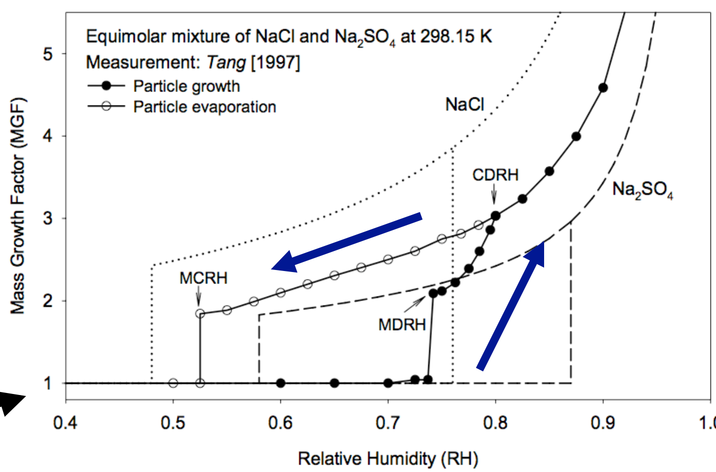
- Compatible with GOCART, MADE/SORGAM, MOSAIC, and MAM aerosol models as of v3.5
- Compatible with Goddard shortwave scheme and RRTMG shortwave and longwave schemes
- Evaluating aerosol size, number distribution, and composition against measurements is essential before calculating optical properties: *If garbage is going into the module, then garbage will come out*

Importance of Aerosol Water

- Aerosol water will have a big impact on optical properties



- Uptake of water by aerosols depends on relative humidity (RH); predictions of RH need to be examined when evaluating aerosol direct radiative effects
- Composition affects water uptake: hydrophobic vs. hydrophillic aerosols
- Aerosols models have different methods of computing aerosol water
  - **GOCART:** Petters and Kreidenweiss (2007)
  - **MADE/SORGAM:** diagnosed
  - **MOSAIC:** prognostic specie that accounts for hysteresis effect (currently being updated for OIN species)
  - **MAM:** prognostic specie, Kohler theory



Refractive Indices

- Refractive index of a substance is a dimensionless number that describes how light propagates through a medium
- Refractive indices in models based on literature values derived from laboratory experiments, vary with wavelength for some aerosol compositions

Default Values for SW Radiation in WRF (users can change)

	real part		imaginary part
BC =	1.850	+	0.71i (all λ)
OM =	1.450	+	0.00i (all λ)
SO_4 =	1.468	+	1.0e-9i (300 nm), small λ dependence
NH_4NO_3 =	1.500	+	0.00i (all λ)
NaCl =	1.510	+	0.866e-6i (300 nm), small λ dependence
dust =	1.550	+	0.003i (all λ), depends on type of dust
H_2O =	1.350	+	1.52e-8i (300 nm), small λ dependence

greater the # $\rightarrow$ more absorption

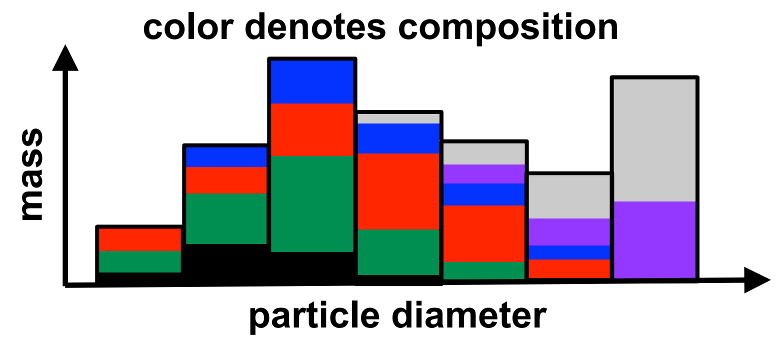
similar relationships for LW radiation

- On-going research:
  - secondary organic aerosols (SOA) may be absorbing at near-UV range
  - how to handle “brown carbon”

Mixing Rules for Mie Calculations

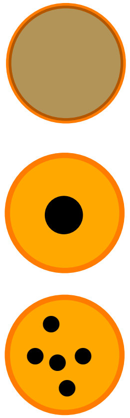
Prior to the Mie calculations, refractive indices need to be averaged among the compositions in some way for discrete size ranges of the aerosol size distribution.

All particles within a size range assumed to have the same composition, although relative fraction can differ among size ranges.



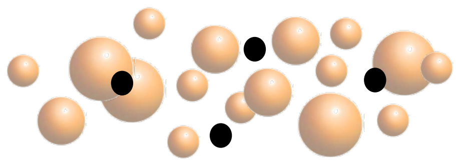
Currently three choices in WRF:

- **Volume Averaging:** averaging of refractive indices based on composition
- **Shell-Core**: black carbon core and average of other compositions in shell (Ackermann and Toon, 1983; Borhren and Huffman, 1983)
- **Maxwell-Garnett:** small spherical randomly distributed black carbon cores in particle (Borhren and Huffman, 1983)

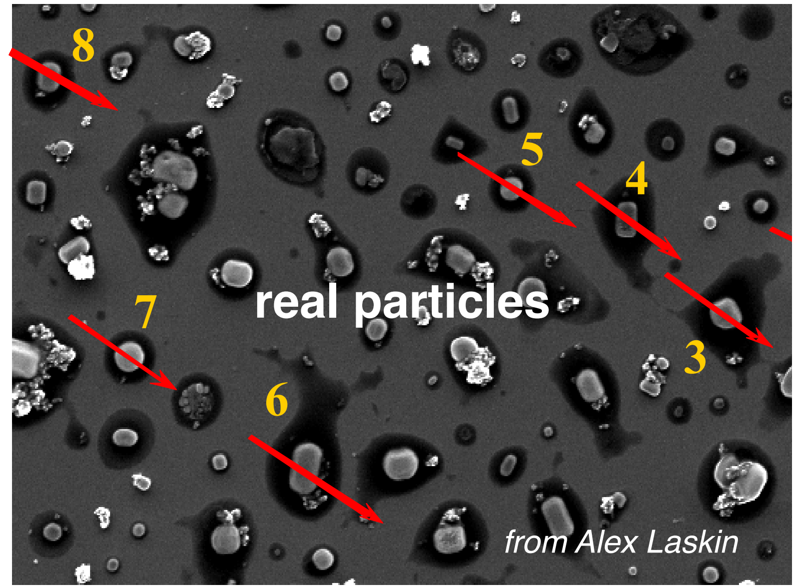


Mie Calculations

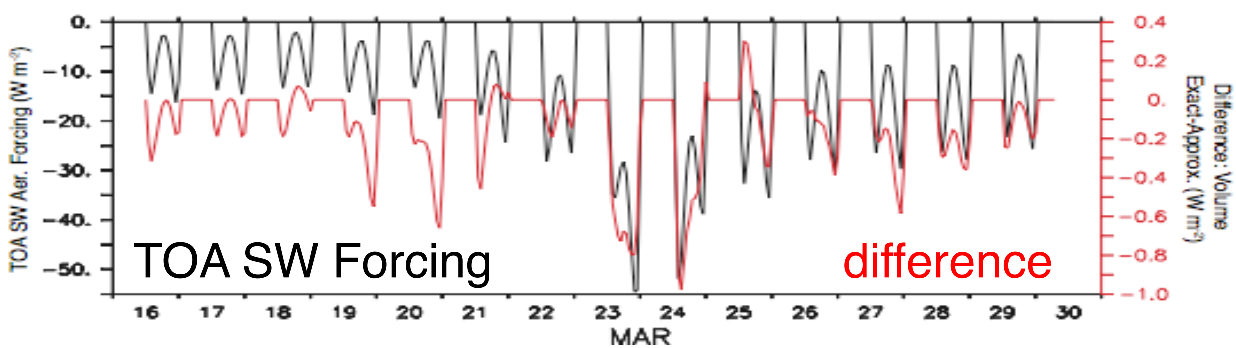
- The Mie solution to Maxwell's equations describes the scattering of radiation by a sphere, used to obtain AOD_l, ω_o, and g



- Aerosols are rarely spheres; however, aged aerosols become more "sphere-like"
- Several "standard" codes available and one is included in WRF
- Mie codes can be computationally expensive, so an approximate version (*Ghan et al*. JGR, 2001) is also available

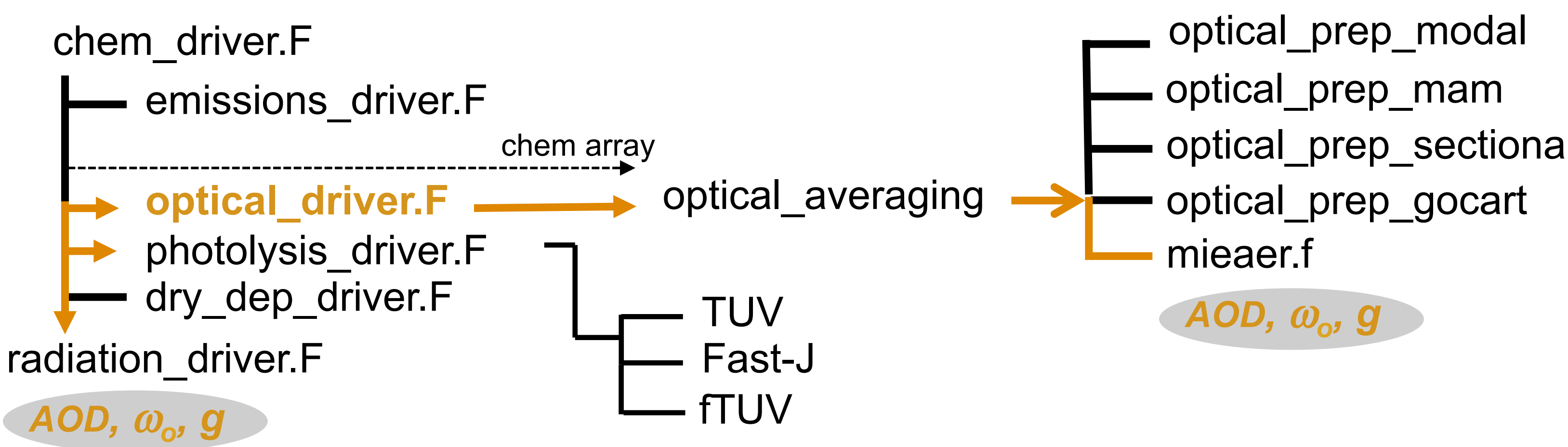


other codes available to handle more complex morphology, but not clear if it is really necessary



Coding Structure

Generic Aerosol Optical Properties Module for WRF-Chem



Example of making the code more generic and interoperable:
optical property is calculated in one routine rather than in each aerosol model

Assumptions of Optical Property Module

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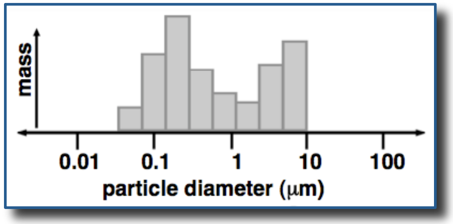
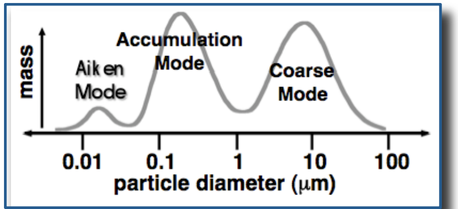
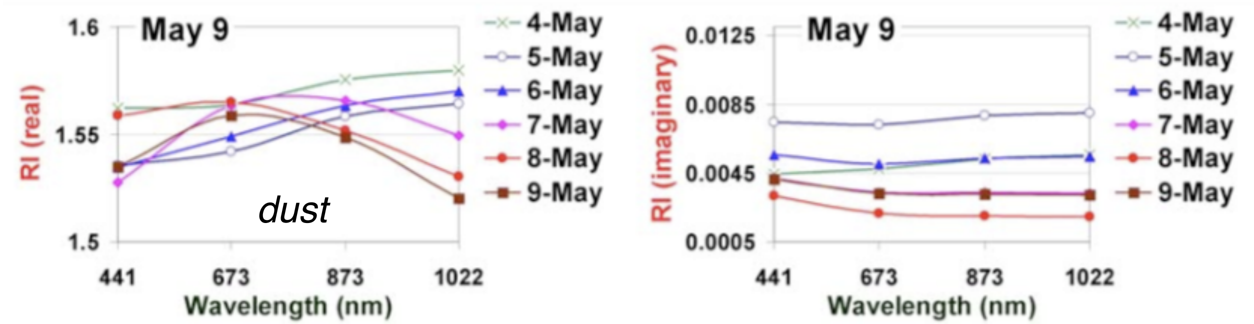
- Interfaces with GOCART, MADE/SORGAM, MAM, and MOSAIC, but linking to other aerosol models should be relatively easy
- **Sectional** (MOSAIC): tested only with 4 and 8 size bins should work if additional size bins are specified



- **Modal** (MADE/SORGAM, MAM): maps the used size modes into 8 sections



- **Bulk** (GOCART): converts bulk mass into assumed distribution, then divides mass into 8 sections
- Note: Refractive indices may need updating
  - Range of values reported in the literature
  - Wavelength dependence of refractive indices for some species

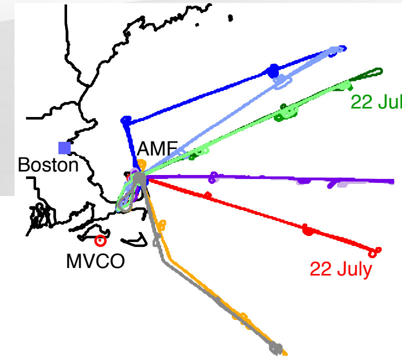


from Prasad and Singh, JGR, 2007

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

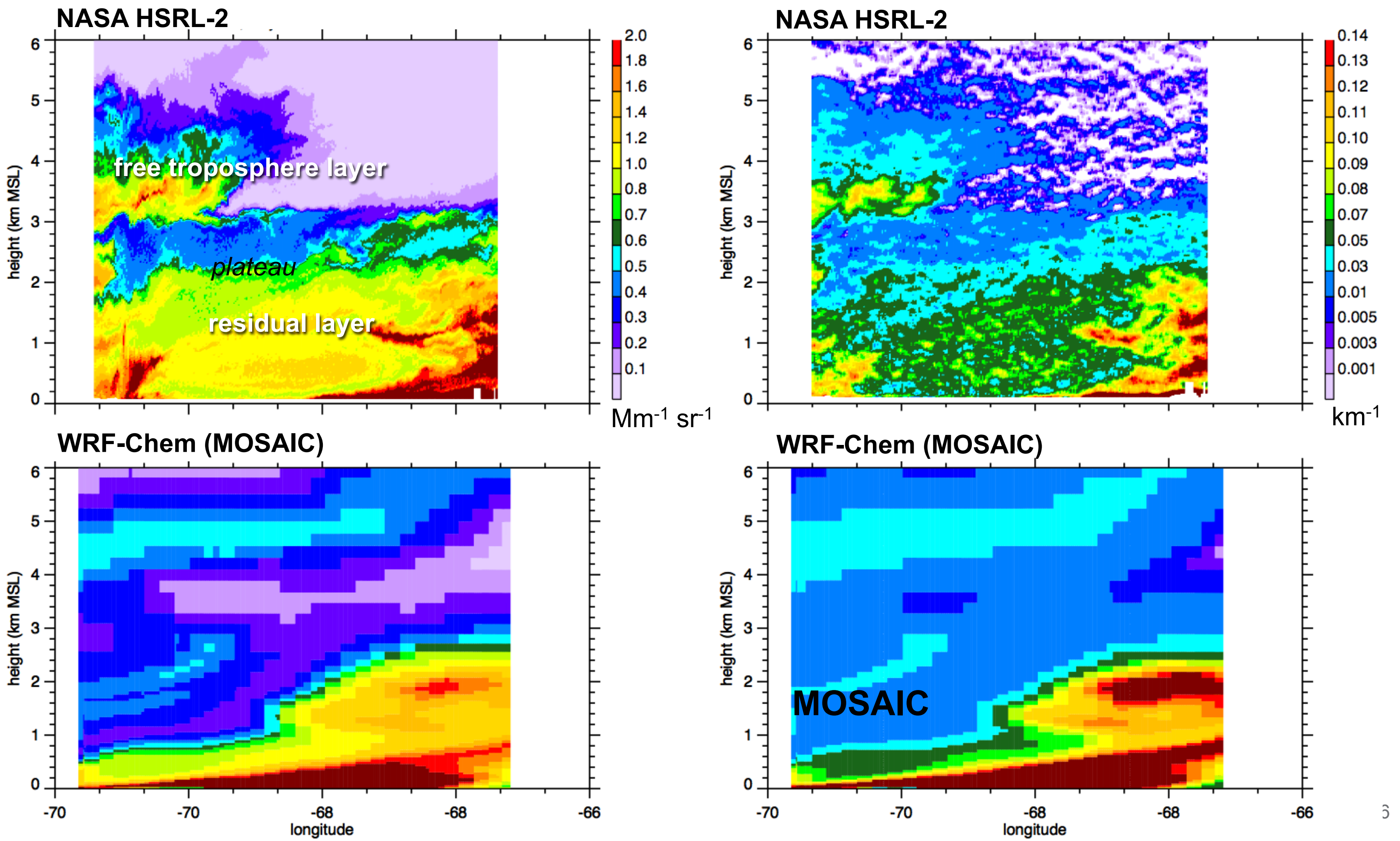
Example: Evaluating Extinction Profiles

from Fast et al. (2016)

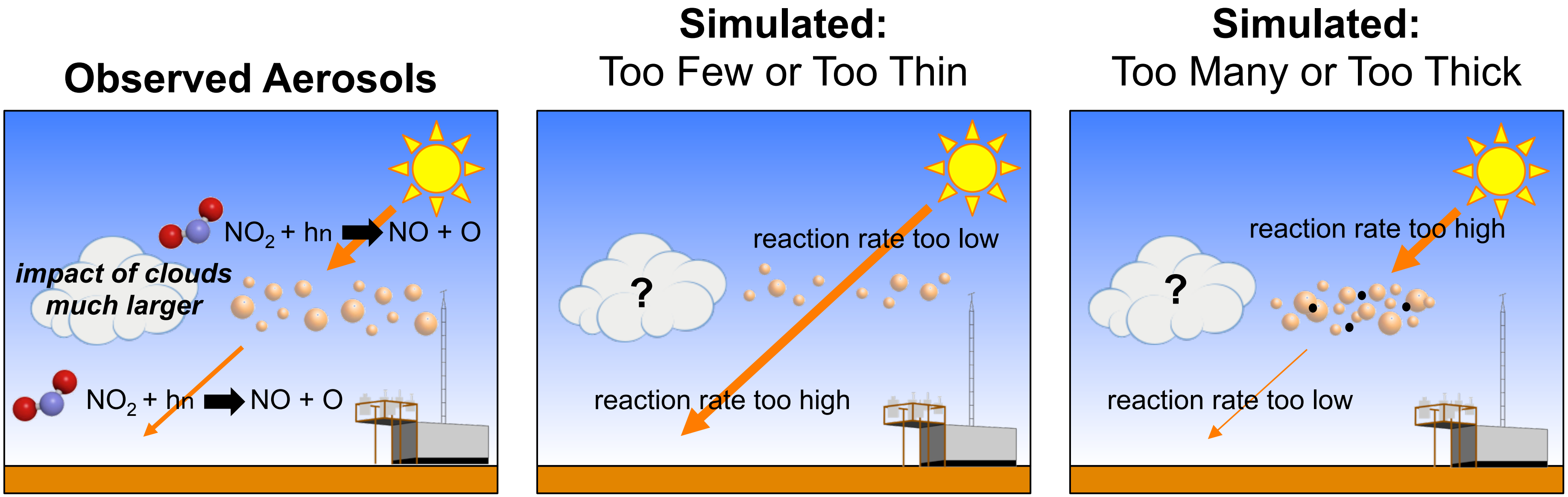


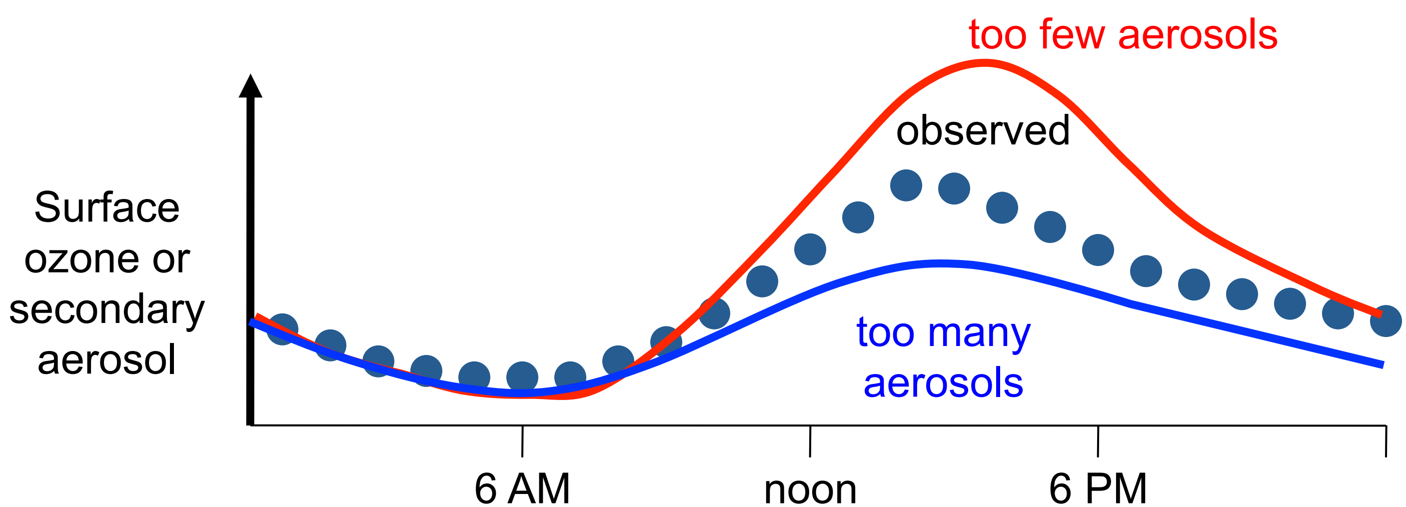
Aerosol Layers during the 2012 TCAP Campaign

Backscatter (532 nm) | **Extinction (532 nm)**



Impact of Aerosols on Chemistry



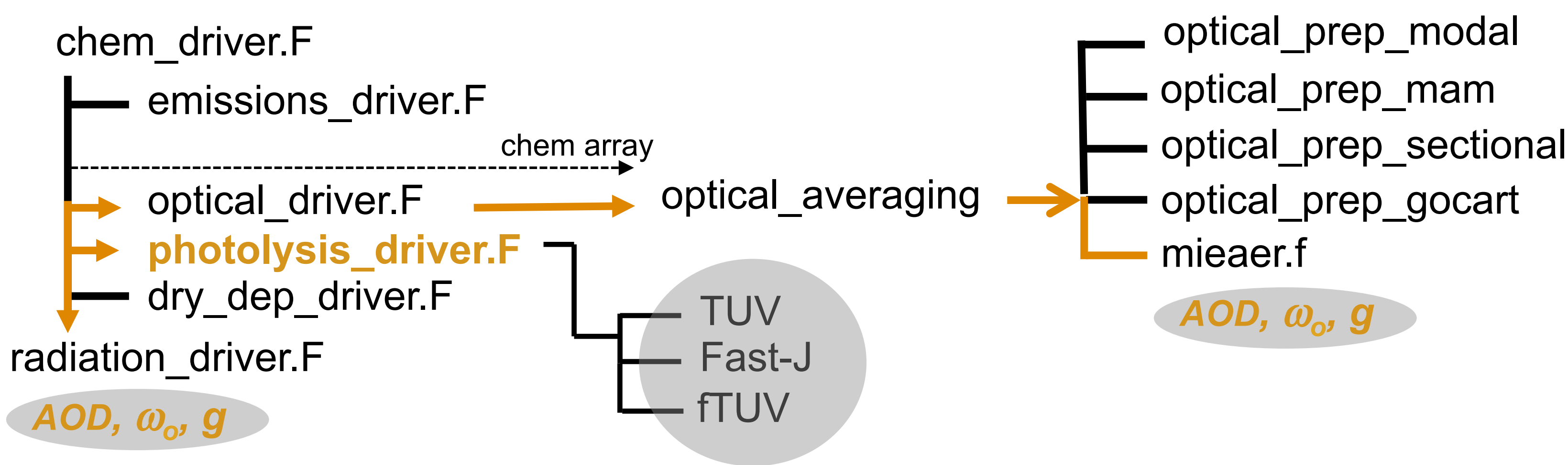


errors could impact simulated concentrations the next day

How Aerosols Affect Photolysis Rates

Aerosols → Photolysis Rates → Photochemistry

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

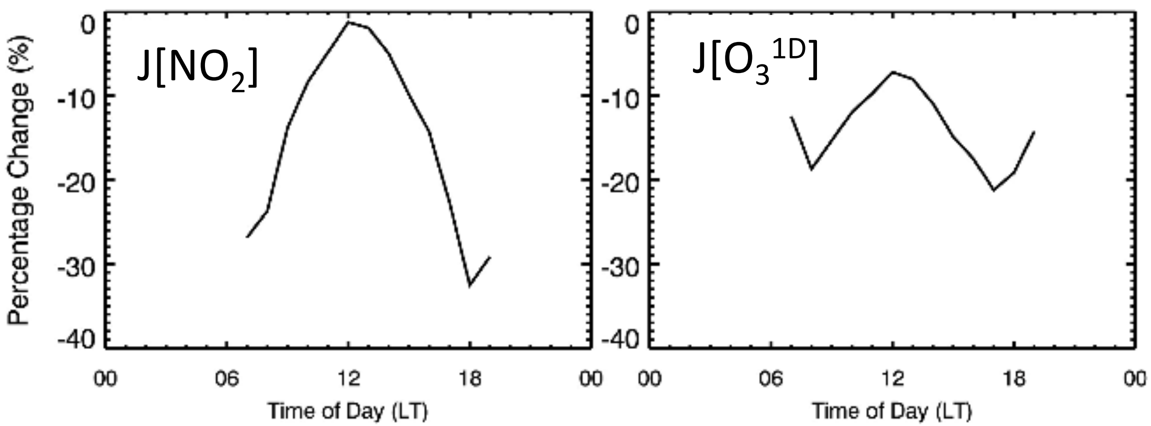


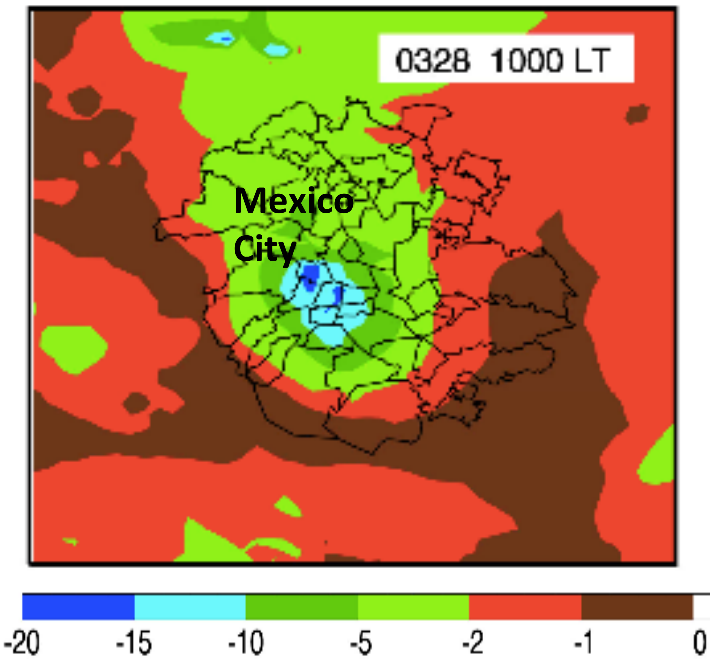
- Fast-J: uses AOD, ω_o, and g computed by module_optical_averaging.F
- FTUV: was updated in v3.6 to use AOD, ω_o, and g computed by module_optical_averaging.F

Example: Impact of Aerosols on Photolysis

from *Li et al.* ACP (2011)

Aerosol effects on surface photolysis and ozone in Mexico City





O_3 percentage change (%)

- Decrease in $J[NO_2]$ and $J[O_3{}^{1D}]$ values during the day
- Decrease in surface ozone concentrations by 5-20% within the Mexico City

Example: Impact of Aerosols over Europe

from *Forkel et al.* ACP (2012)

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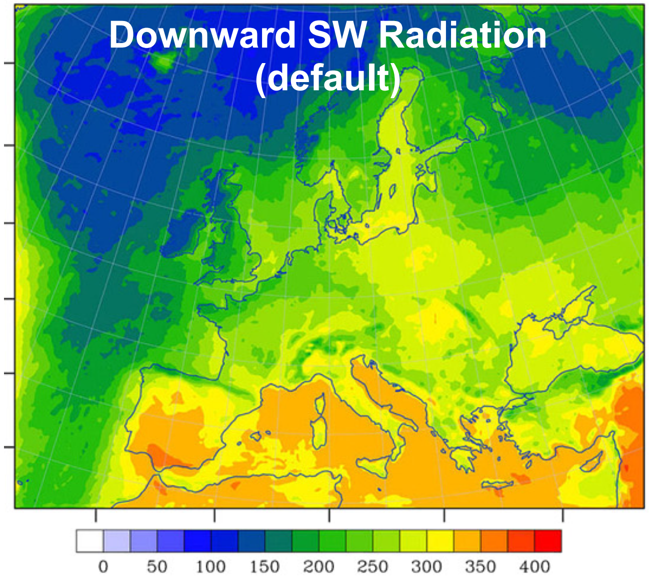
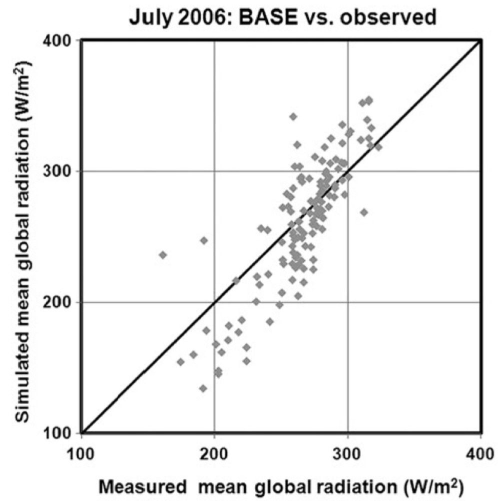
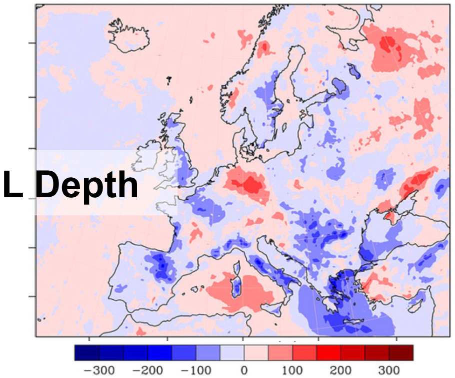
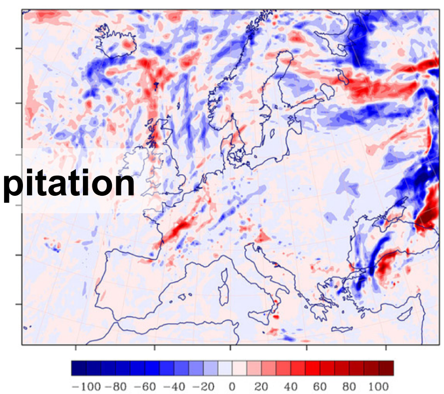


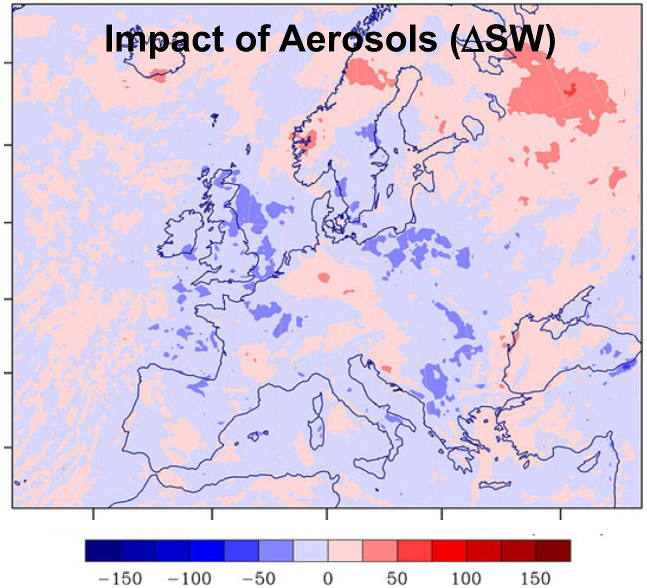


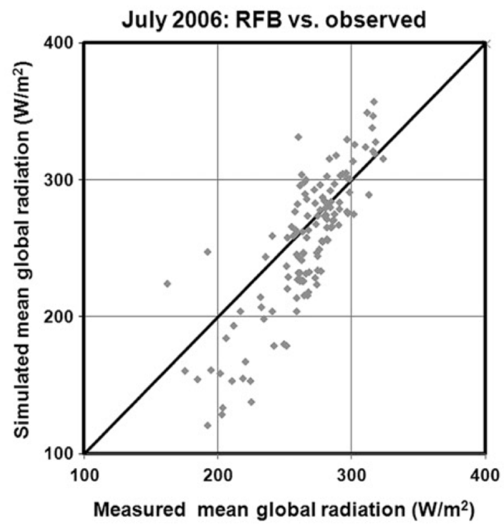


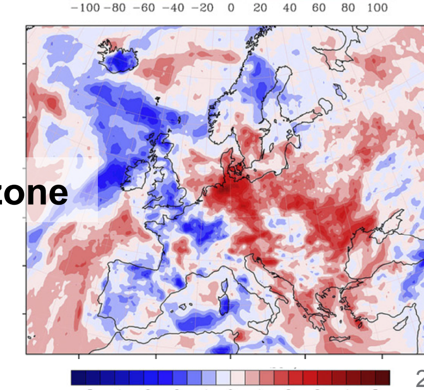
Δ PBL Depth



Δ Precipitation







Δ Ozone

Settings in namelist.input

Important Parameters:

- ra_sw_physics = 2 aerosols affects radiation computed by Goddard scheme
- ra_sw_physics = 4
- ra_lw_physics = 4

aerosols 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, MAM, and MOSAIC options

Direct Effects:

- Simulations with aer_ra_feedback = ON or OFF can be used to quantify direct effects, but differences in clouds complicates interpretation
  - Useful to add code that computes radiation with and without aerosols and with and without clouds (either directly in the code or computed off-line)
  - Or work with small perturbations in aerosol fields

Future Capabilities

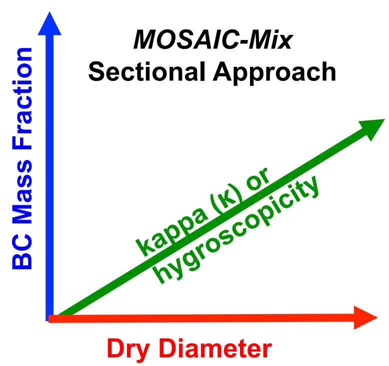
Research – Possibly in Upcoming Releases of WRF:

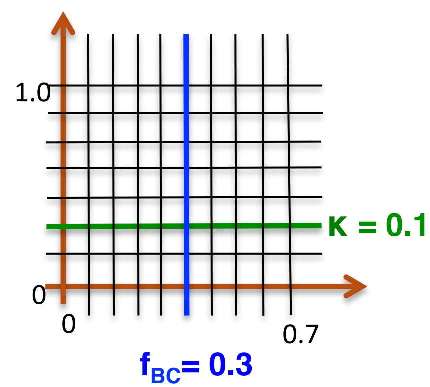
- Different refractive indices organic aerosol components
- More computationally efficient Mie calculations
- More detailed treatment of optical properties of organic aerosols including treatment for "brown carbon"
- Code to handle aerosol model with external mixtures

Current MOSAIC **Sectional Approach**

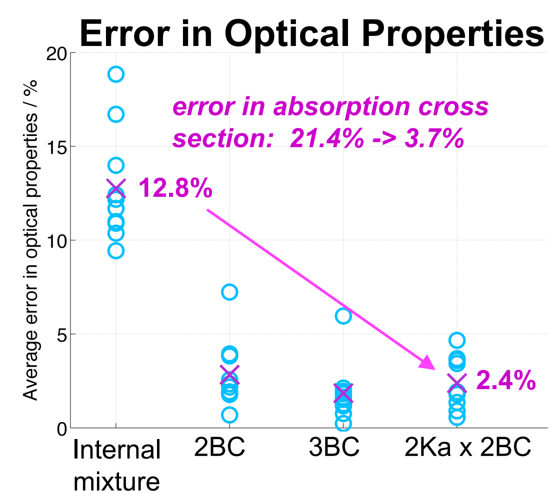
In each size bin, all particles have same BC mass fraction and same kappa

Dry Diameter



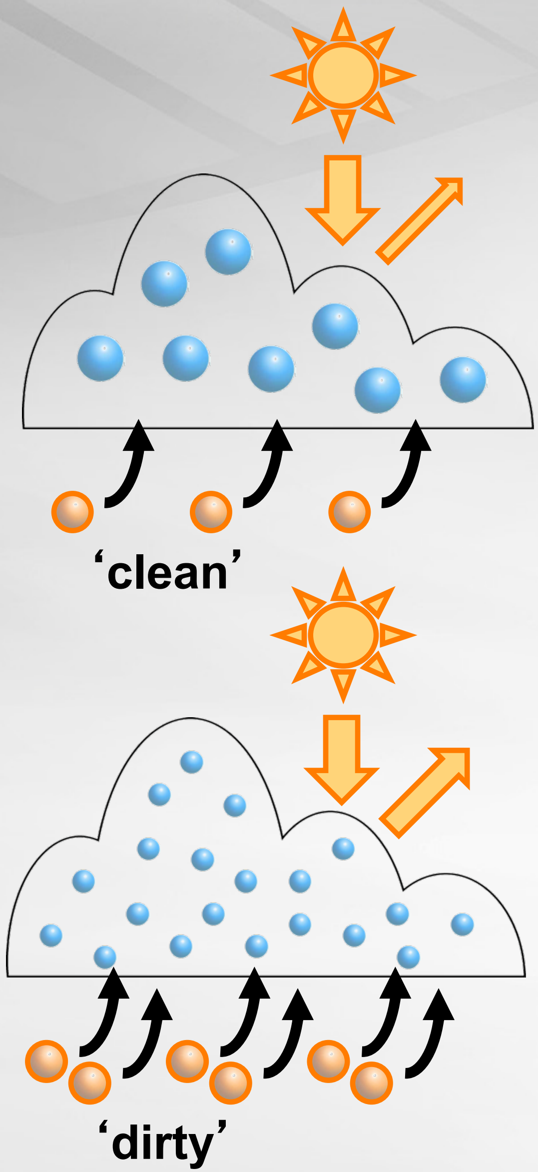


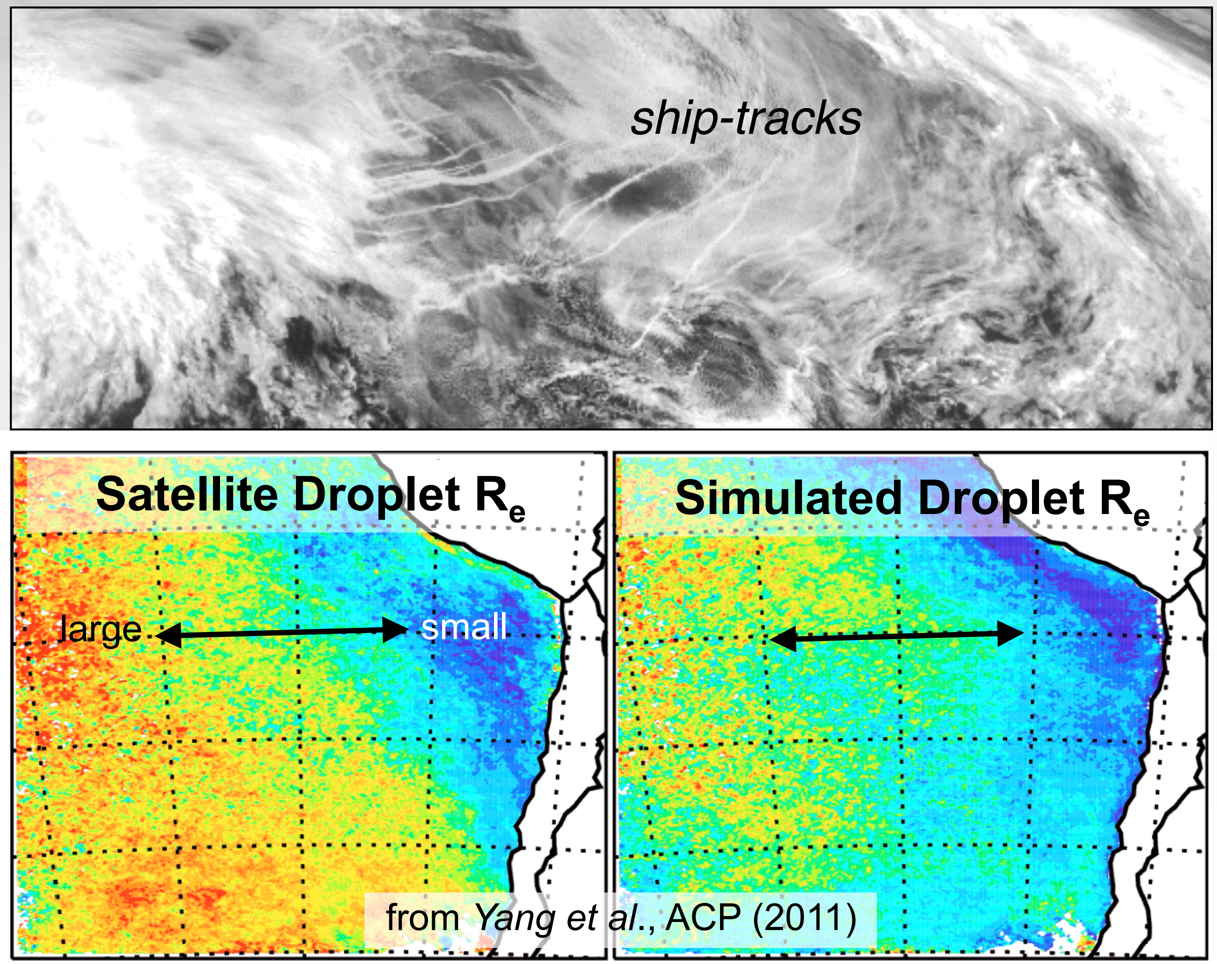
identify optimal bin boundaries compared to explicit calculations



Ching et al., 2016, JGR
also see Matsui et al., 2014, ACP

Part 2: Aerosol Indirect Effects





The number of activated aerosols affects the cloud drop size distribution, and consequently cloud albedo and radiation budget

Aerosol-Cloud Interactions in grid-scale clouds

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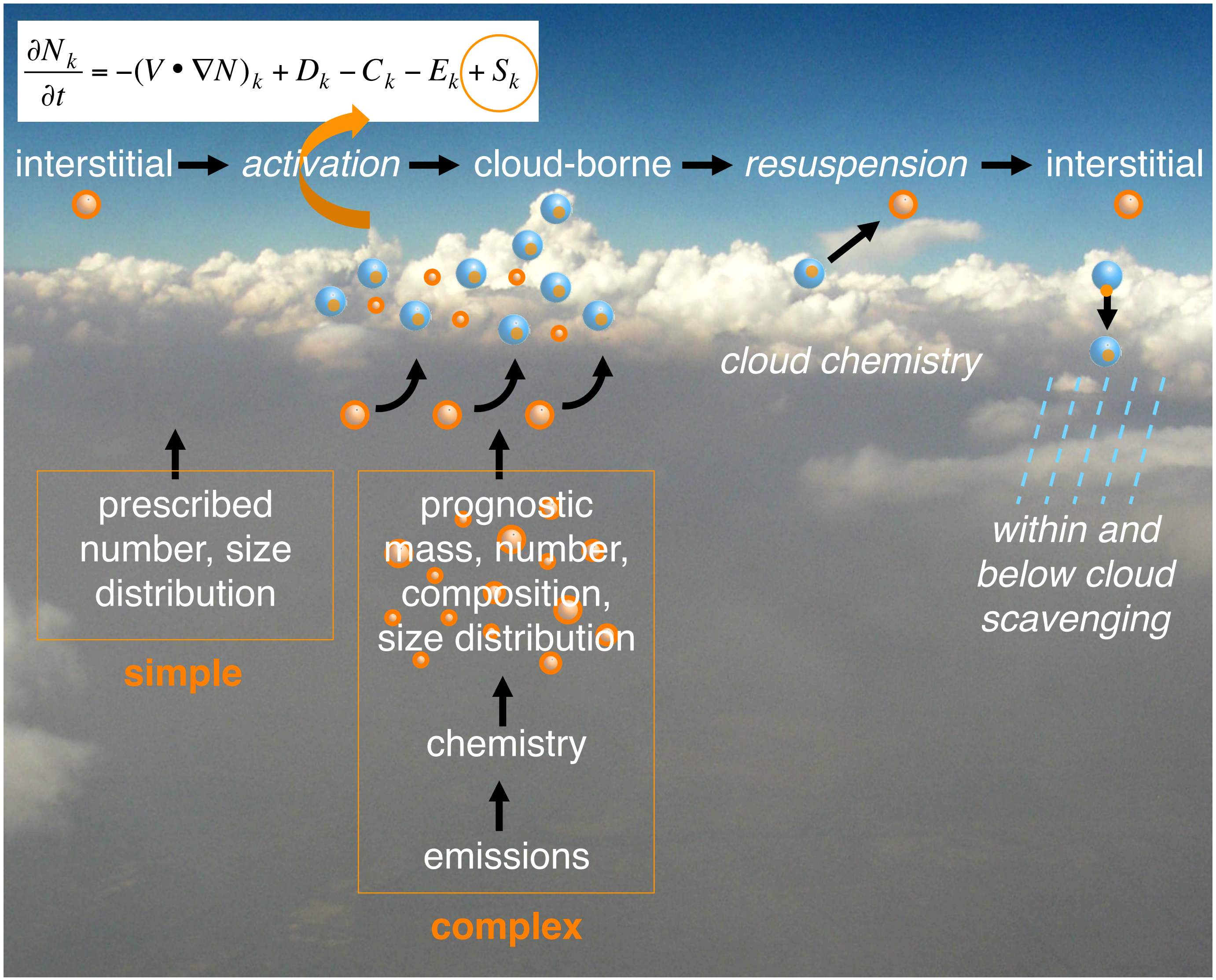
General Description and Assumptions

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



Simple:

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

Complex:

- chem_opt = 9-12, 32, 34, 35, 41-43, 132, 202, 203, 503, 504, 601, 611
- progn = 1
- naer = ignored

coupled to 2 microphysics schemes: Lin and Morrison

Flow Chart

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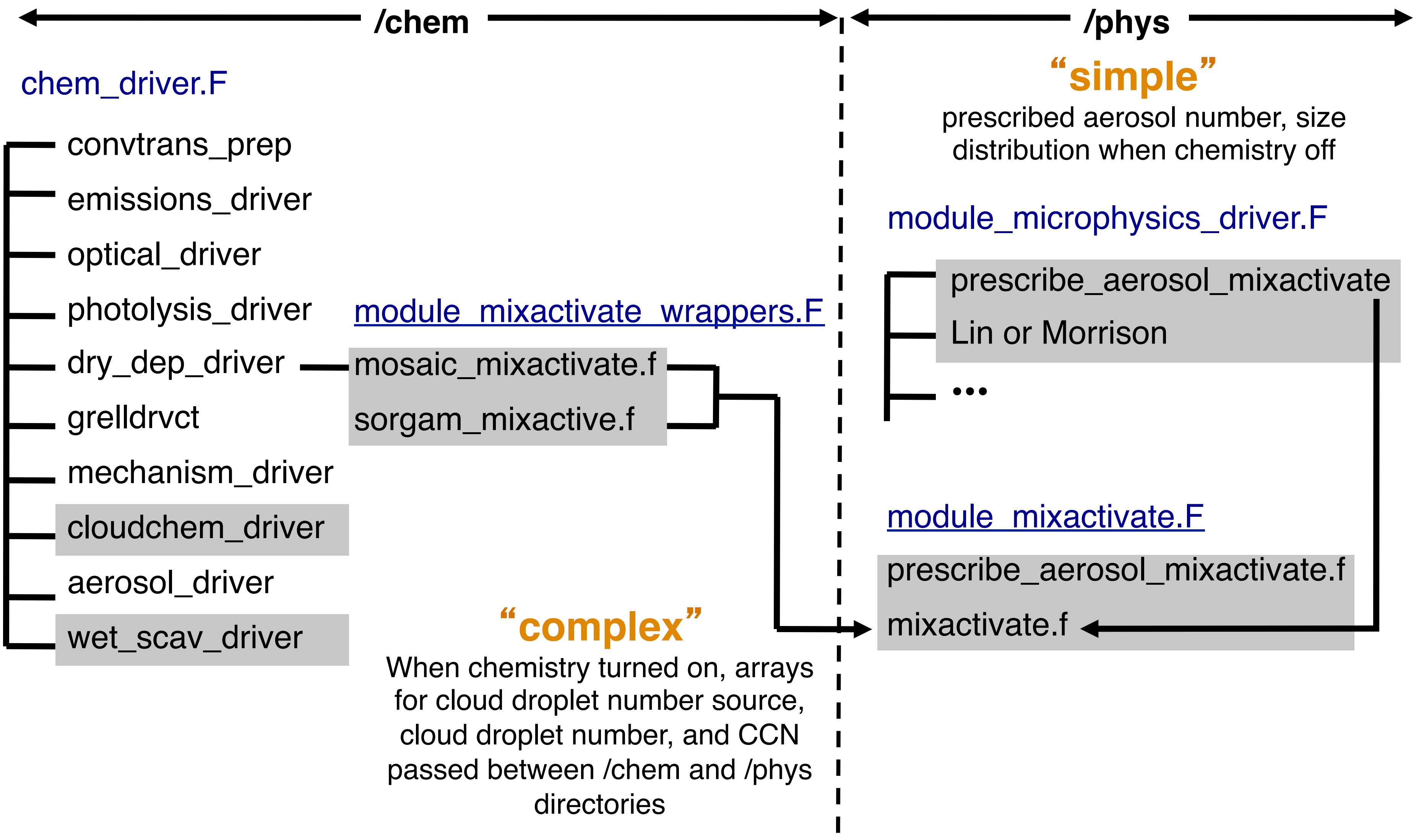


Aerosol Species

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

interstitial		cloud-borne		interstitial
so4_a01	*activation* →	so4_cw01	*resuspension* →	so4_a01
so4_a02	"growing cloud"	so4_cw02	"shrinking cloud"	so4_a02
…	cldfra - cldfra_old > 0	…	cldfra_old > cldfra	…
no3_a01		no3_cw01		no3_a01
no3_a02		no3_cw02		no3_a02
…		…		…
num_a01		num_cw01		num_a01
num_a02		num_cw02		num_a02

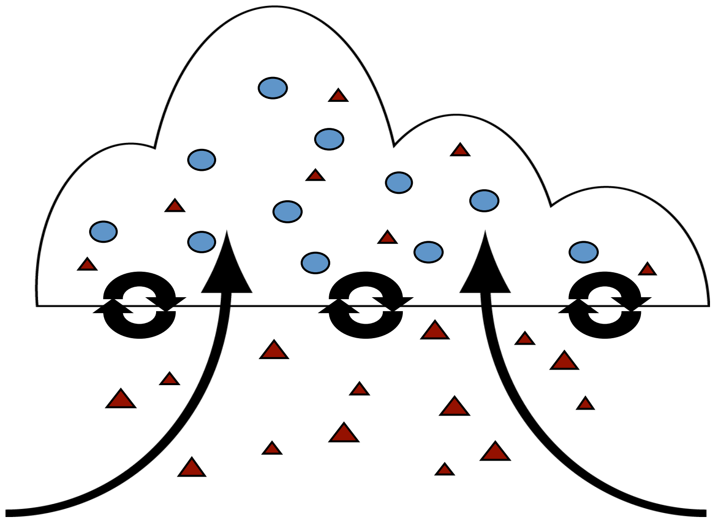
8 bins x 12 species + hysw + water = **112**

8 bins x 12 species = **96**

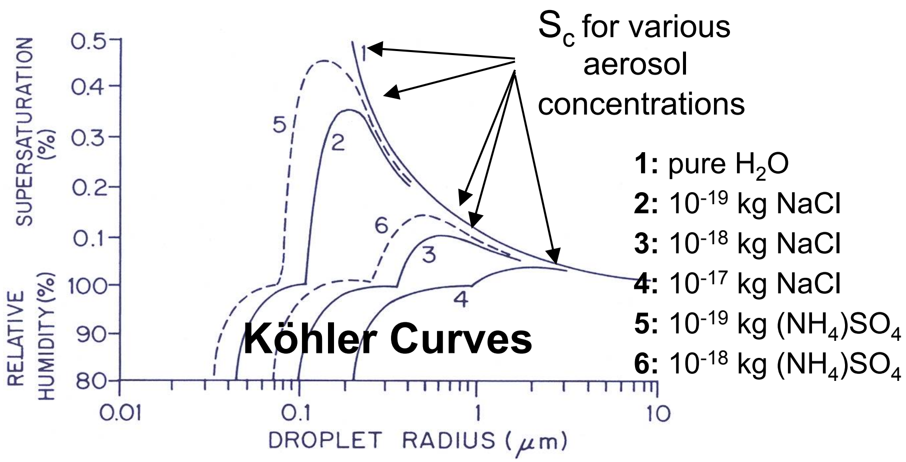
computational expense associated mostly with transporting scalars

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

Activation



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



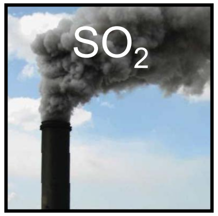
Activate.f computes activation fraction for mass and number for each bin/mode. Inputs include mean vertical velocity, *wbar*, and s of the turbulent velocity spectrum, *sigw*.

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.

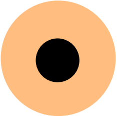
For each vertical velocity, peak S_{max} depends on aerosol size and composition [*Abdul Razzak and Ghan,* 2000, 2002]. Activation fraction based distribution of $\mathbf{S_c}$ of the bin/mode - simply a fraction of aerosol mass or number in the bin/mode having $\mathbf{S_c}$ < $\mathbf{S_{max}}$

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 *hydrophobic*
  - 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
  - hygro_na_aer = 1.16 *hydrophilic*



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



Coating not taken into account

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

Cloud Condensation Nuclei

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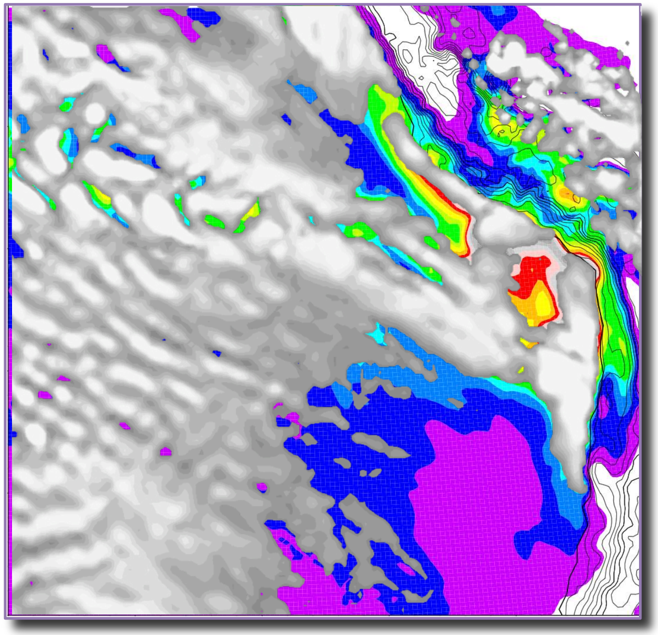
- CCN: number concentration of aerosols activated at a specified super-saturation
- Diagnostic quantity, varies in space and time (can be measured)
- Computed in module_mixactivate.F

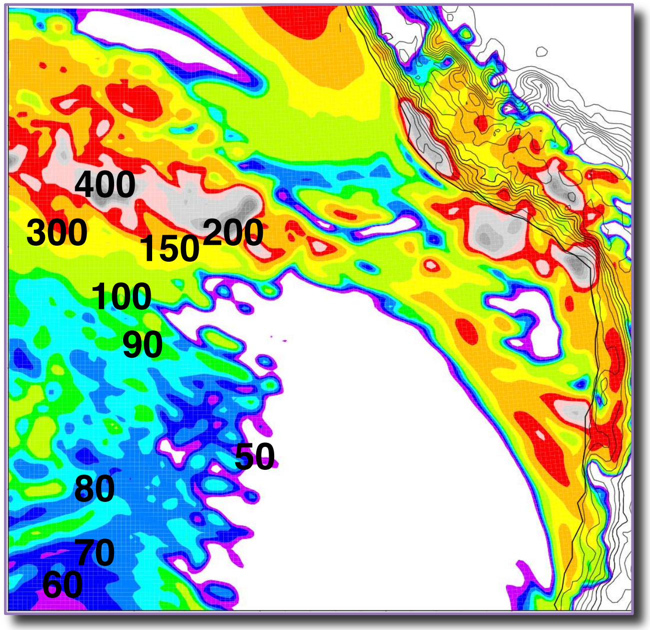
  at 6 super-saturations (.02, .05, .1, .2, .5, and 1%) that correspond

  to CCN1, CCN2, CCN3, CCN4, CCN5, CCN6 in Registry

AOD (600 nm) and COD



CCN at 0.1% SS (# cm^{-3})



example from VOCALS-Rex: southeastern Pacific marine stratocumulus

Aqueous Chemistry

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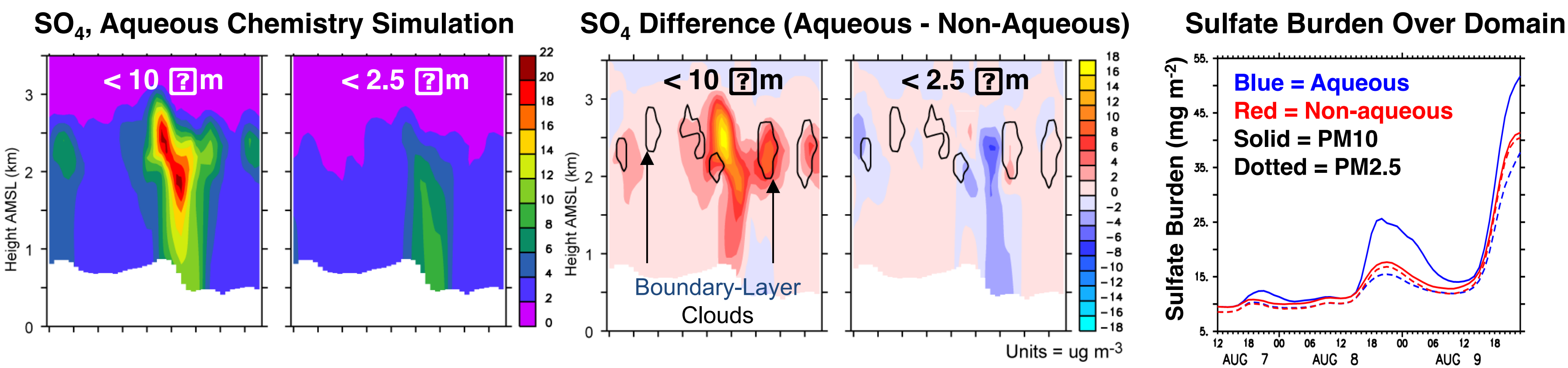
- Bulk cloud-chemistry module of Fahey and Pandis (2001) compatible with MOSAIC and MADE/SORGAM (cloudchem_driver.F)
- Chemistry in cloud drops, but not rain drops
- Oxidation of S(IV) by H_2O_2, O_3, trace metals, and radical species, as well as non-reactive uptake of HNO_3, HCl, NH_3, and other trace gases
- Bulk mass changes partitioned among cloud-borne aerosol size bins, followed by transfer of mass & number between bins due to growth

Vertical Cross-Section Though Power Plant SO_2 Plume

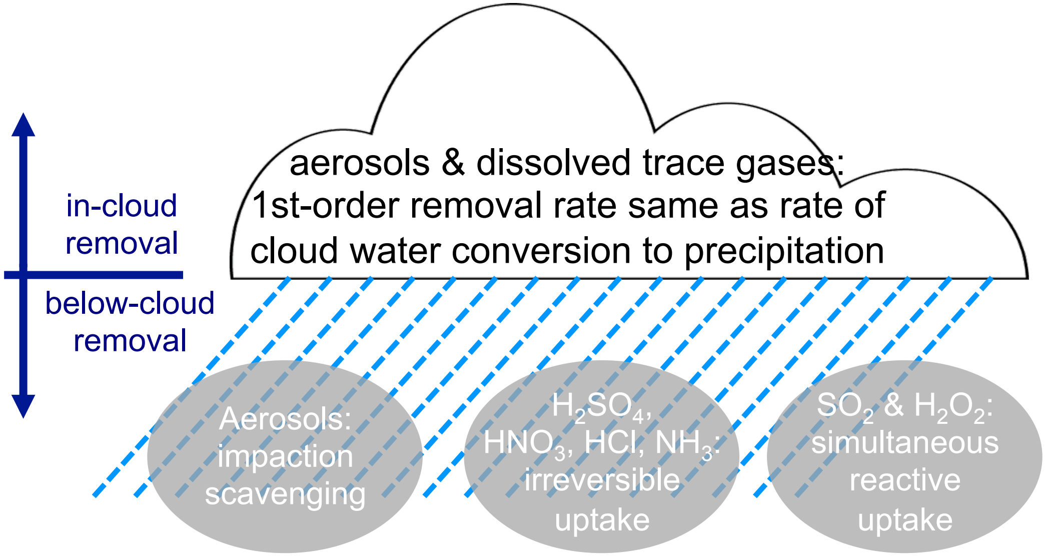


aqueous chemistry results in more SO_4 mass in coarse mode

Wet Removal

- Cloud-borne aerosols and trace gases are collected by both grid-scale and convective precipitation (rain, snow, graupel)

- cloud-borne aerosols are explicit, while the fraction of trace gas that is dissolved in cloud water is calculated in the cloud chemistry module



- scavenged aerosols and gases instantly removed *Easter et al.* (2004); aerosols are not resuspended by evaporating rain

- In MOZART based packages, the washout of trace gases is based on Neu and Prather (2012), and updated solubility coefficients are used for organic gases

Cloud Droplet Number

- converted Lin et al. microphysics scheme to a two-moment treatment (mass & number), in addition to adding impact of aerosols on droplet #
- Morrison microphysics is a two-moment treatment, so only needed to add code to include the impact of aerosols on droplet #

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

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

qndropsource (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)

Example: Marine Stratocumulus

from *Yang et al.* ACP (2011)

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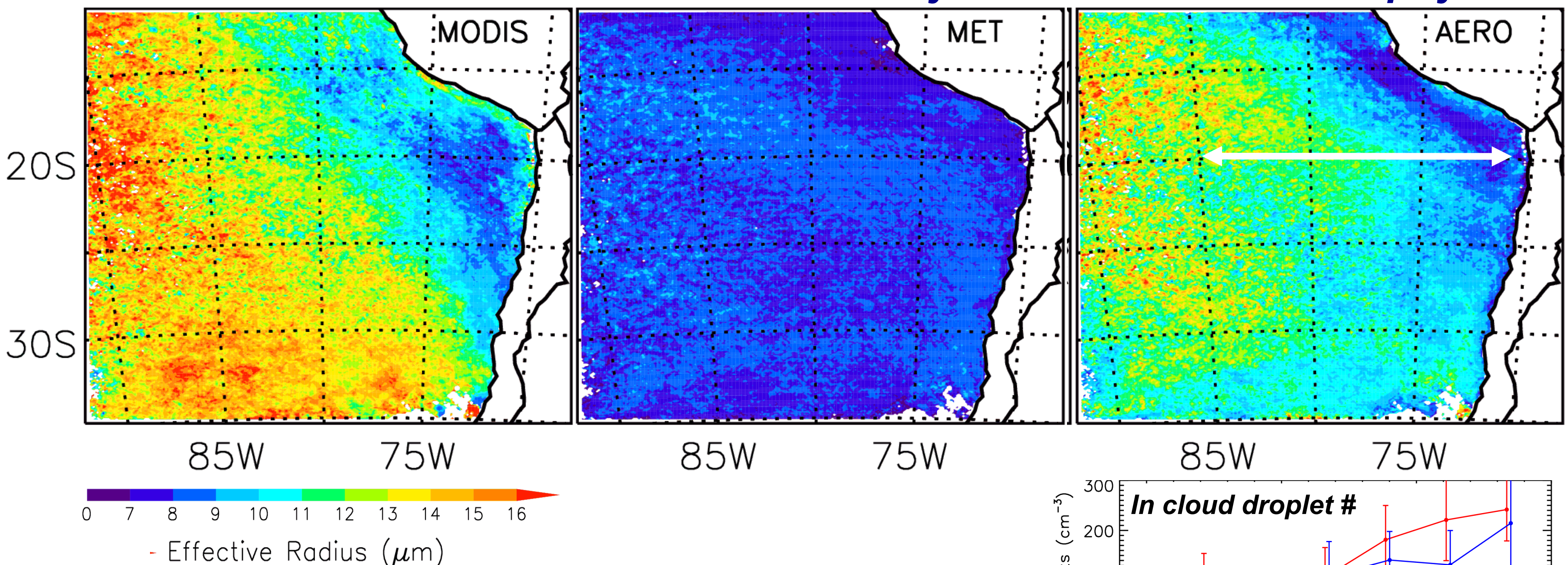
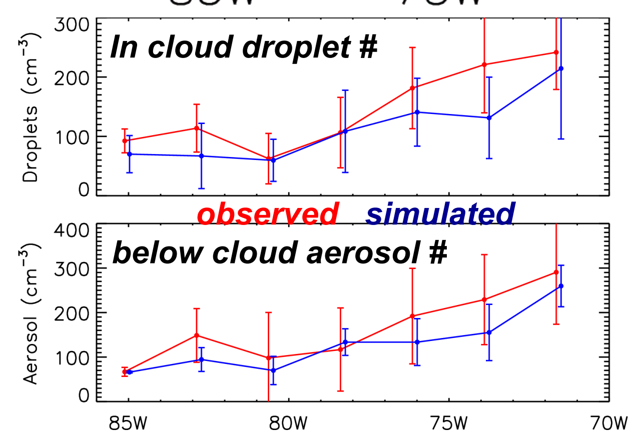
Average Effective Droplet Radius during 2008 VOCALS-REx

MODIS | ***WRF no chemistry*** | ***MOSAIC aerosols and Morrison microphysics***

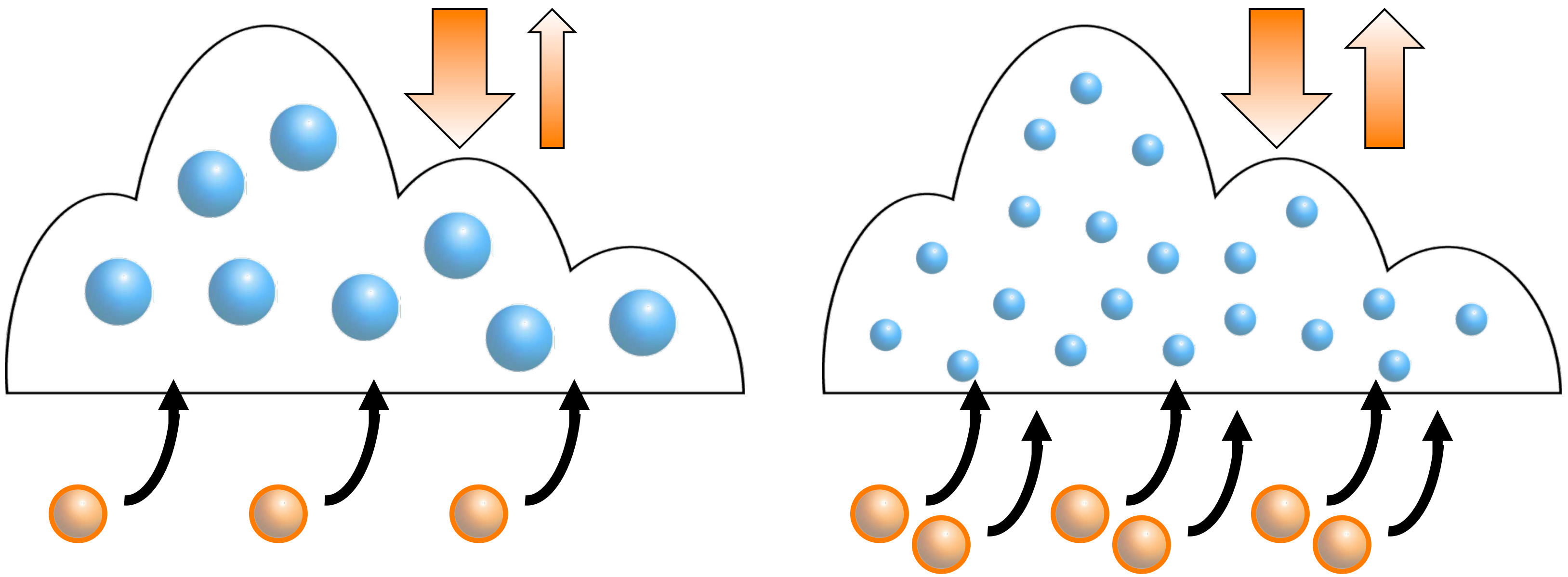




- Yang et al. (2011) used the Morrison microphysics for this case, while Saide et al. ACP (2012) used the Lin microphysics to evaluate cloud-aerosol interactions

First Indirect Effect

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



'clean' 'polluted'

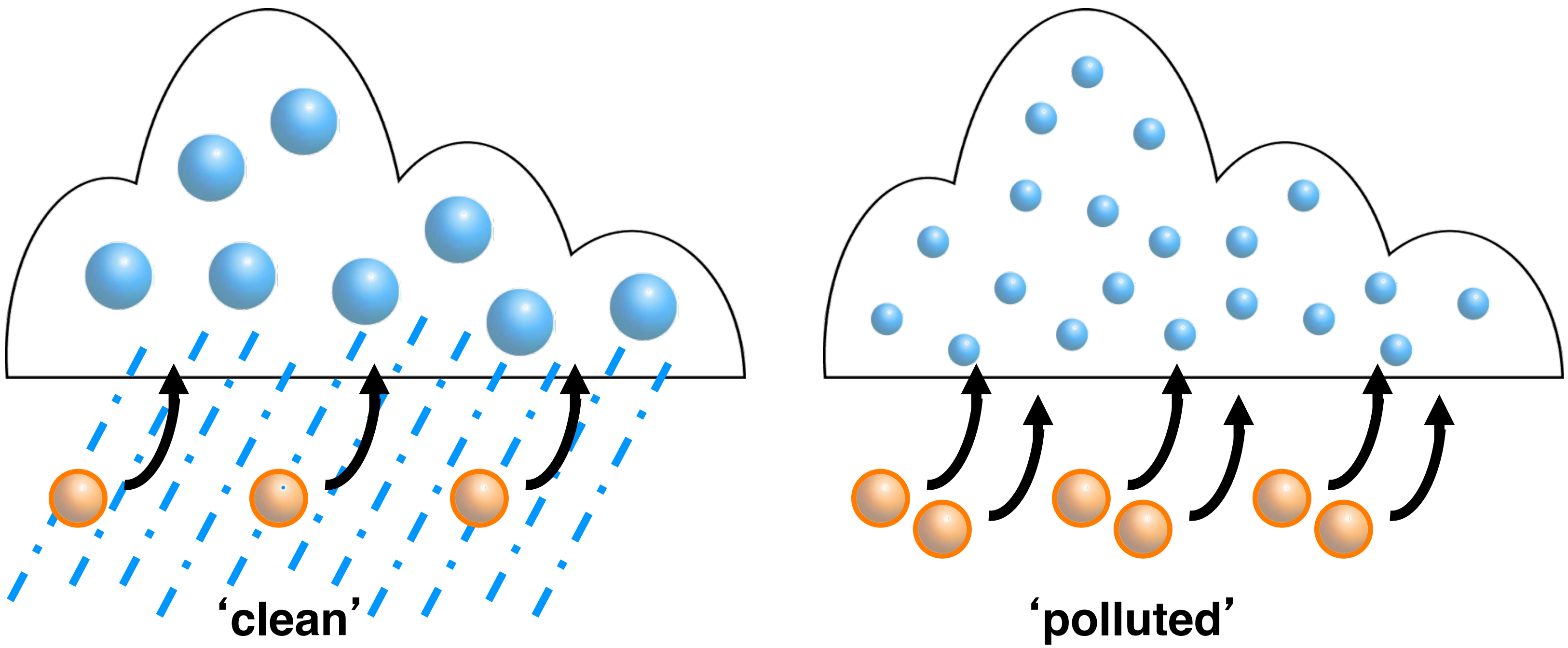
qndrop → gsfcwrad.f → reff → sorad.f → taucld

module_ra_gsfcsw.F effective radius cloud albedo

(subroutines 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



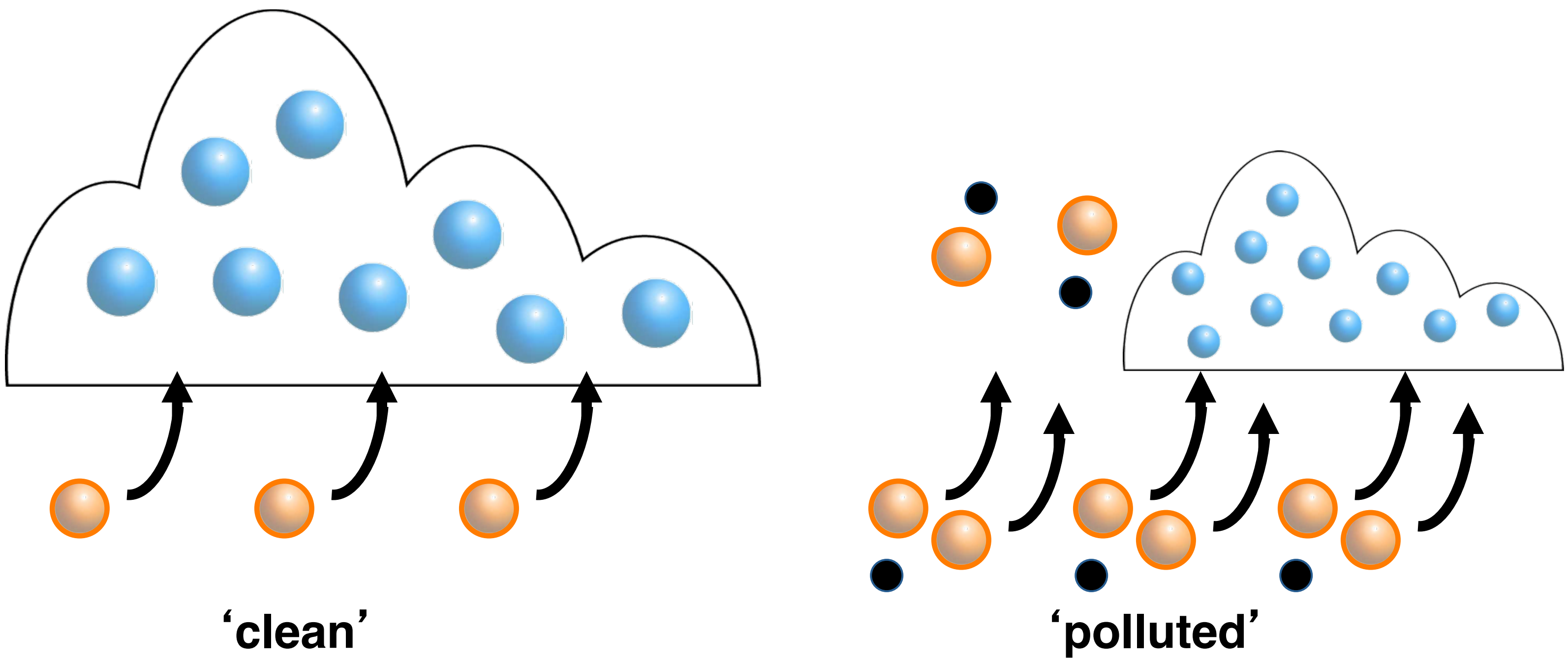
qndrop → cldphy_1d.f → praut → qr → precr

module_mp_lin.F | autoconversion rate | rain mixing ratio

(subroutines for Goddard scheme)

Semi-Direct Effect

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



t, w_o, g → gsfcwrad.f → sorad.f → flx → ttend2d → q tendency

module_ra_gsfcsw.F

solar uv and ir fluxes

heating rate

(subroutines for Goddard scheme)

Settings in namelist.input

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Cloud-Aerosol Interactions for Lin and Morrison Microphysics

- mp_physics = 2, 10
- progn = 1, turns on prognostic cloud droplet number

Simple:

- chem_opt = 0
- naer = specified value

Complex:

- chem_opt = 9, 10, 32, 34, 202, 203, 601, 602 cloud-phase for MOSAIC
  = 11, 12, 35, 41-43, 132 for MADE/SORGAM
  = 503, 504 for MAM
- cldchem_onoff = 1, turns on cloud chemistry
- wetscav_onoff = 1, turns on wet scavenging

CAM5 Physics is Different (1)

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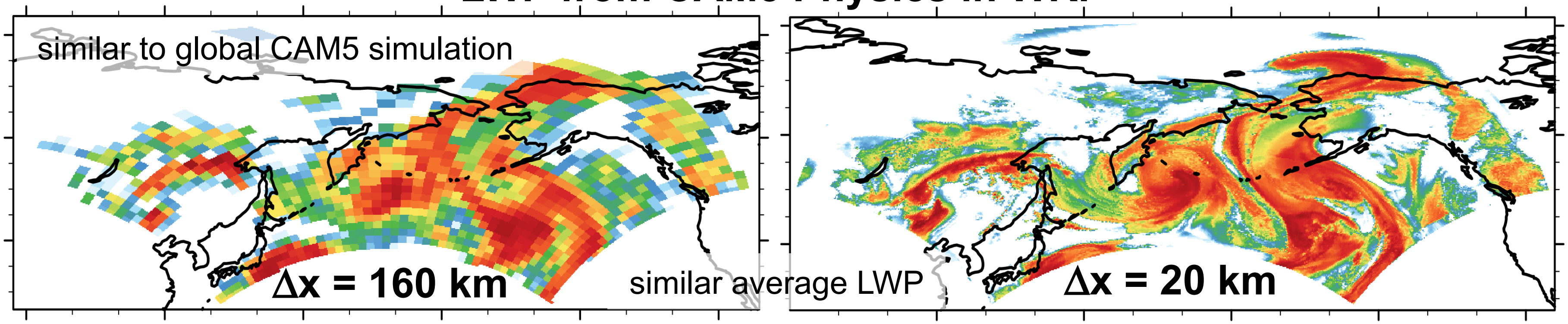
- Cloud-Aerosol Interactions for **Morrison and Gettelman microphysics handled separately**, because
  - CAM5 physics kept as same as possible as in the CESM climate model

LWP from CAM5 Physics in WRF



- Entire CAM5 physics suite must be used when simulating cloud-aerosol interactions in the Morrison and Gettelman microphysics scheme
  - mp_physics=19, cu_physics=7, shcu=physics=2, bl_pbl_physics=9 chem_opt=503, cam_mam_mode=3, CAM_MP_MAM_cpled='true'
- /phys/module_mixactivate.F is not used (activation is done elsewhere), but is conceptually similar to how it is handled in WRF for other models

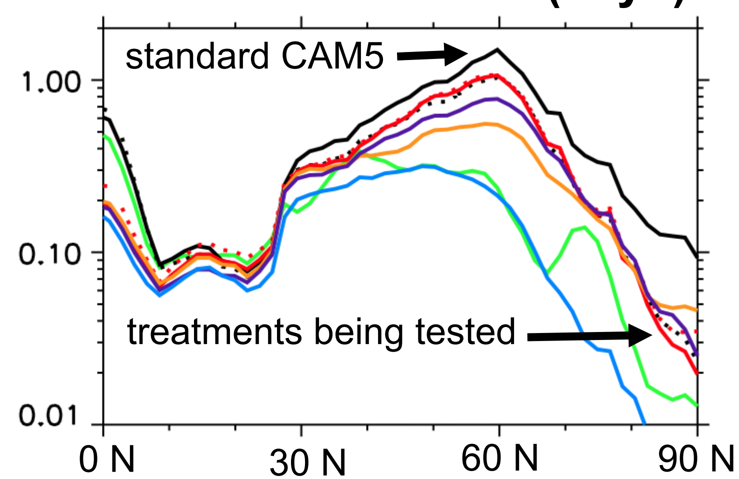
CAM5 Physics is Different (2)

- Morrison and Gettelman microphysics includes treatment of heterogeneous freezing on mineral dust
  - But, there are no ice-borne aerosols
  - Coupling of prognostic aerosols to ice nuclei (IN) not included for other microphysics scheme; the effect of aerosols on cloud droplets will affect ice processes indirectly however

- module_wetscav_driver.F modified to handle MAM aerosols
  - See Wang et al. GMD (2013) for a discussion on wet removal and its uncertainties

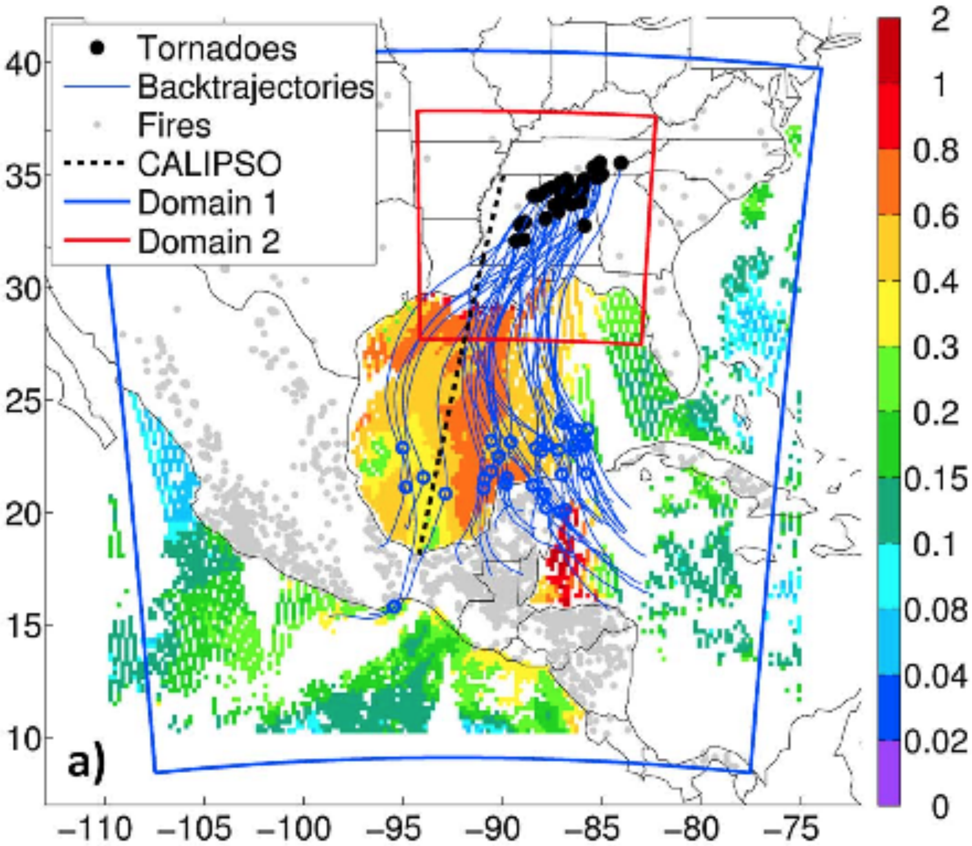
- CAM5 physics in WRF is described in (Ma et al., 2014 GMD) paper.

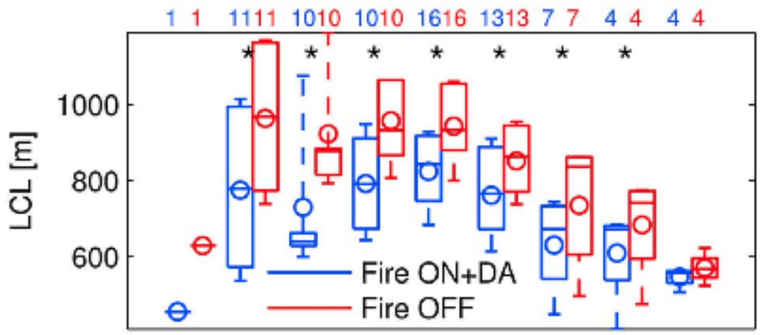
Wet Removal Rate (day^{-1})

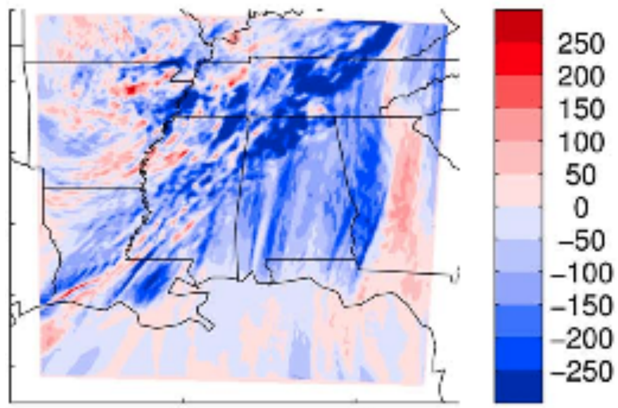


Example: Smoke and Tornado Severity

from *Saide et al.* GRL (2015)







- Inclusion of smoke to an environment already conducive to severe thunderstorm development can increase the likelihood of significant tornado occurrence

Comparing Options

Care Must be Taken in Quantifying Indirect Effects!

Indirect Effects:

- Comparing runs with chem_opt = 8 (without cloud-borne aerosols) with chem_opt = 10 (with cloud-borne aerosols) for MOSAIC coupled to Lin microphysics **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:

- In addition to Abdul-Razaak and Ghan (2000, 2002), other schemes have been used to compute aerosol activation (Foutoukis and Nenes, 2005)
- Works with microphysics only – not cumulus parameterizations so users must be aware of issues associated with **spatial scale**

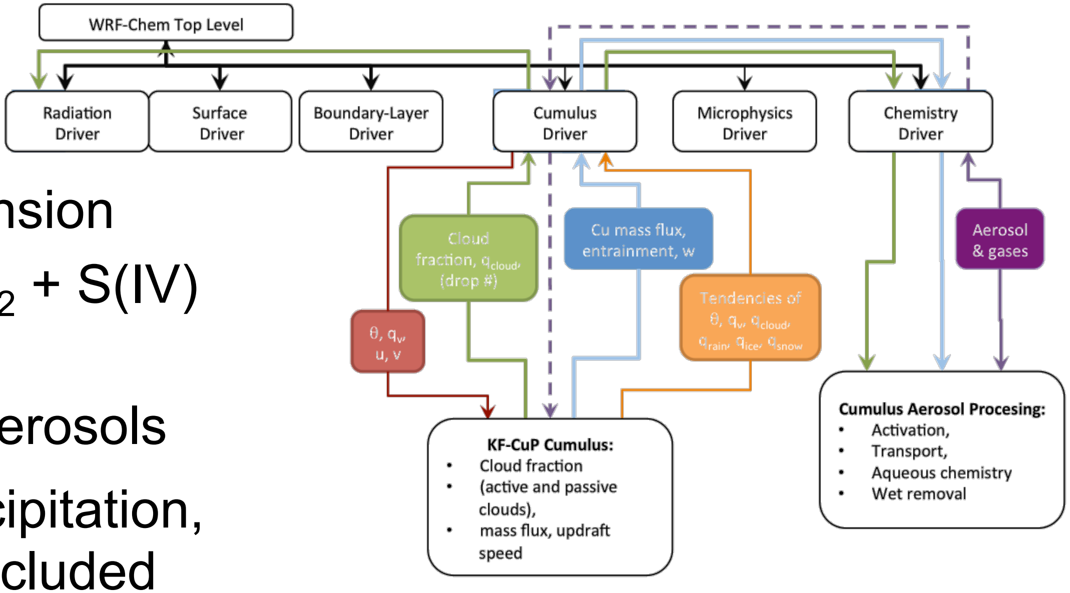
New Option for Parameterized Clouds

Modifications to Kain-Fritsch Cumulus

- Used Cumulus Potential (CuP) approach to improve the simulation of shallow cumuli (Berg et al., MWR, 2013)
- Cloud fraction of both active and passive clouds

New WRF-Chem chemistry package coupled with MOSAIC aerosol – see Berg et al., GMD, 2015

- Vertical transport of gases and aerosols
- Aerosol activation / resuspension
- Aqueous chemistry (gas SO_2 + S(IV) in cloud water)
- Wet removal of gases and aerosols
- Feedbacks to radiation, precipitation, and cloud lifecycle not yet included

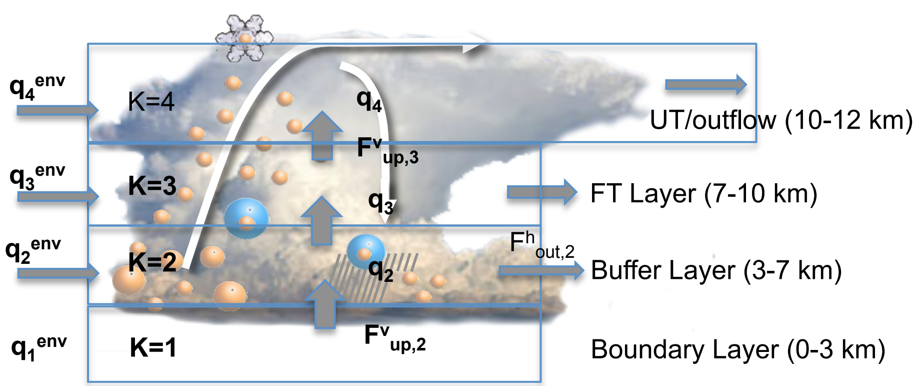


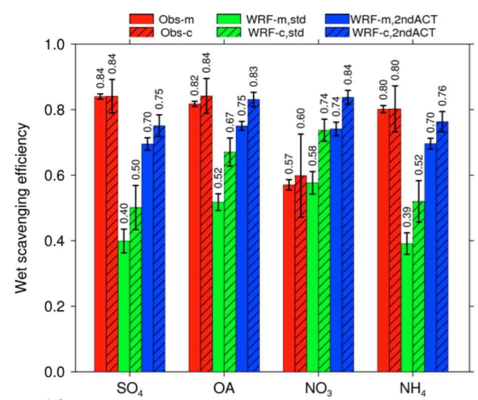
Future Capabilities

Processes Under Development:

- Effects of aerosols in Thompson microphysics (not coupled to aerosol chemistry)
- Other treatments are likely being developed by WRF-Chem users that are not known until they are published
- Resuspension of aerosols from evaporating rain
- Secondary activation
- Ice-borne MOSAIC aerosols and IN treatment

Yang et al., 2015, JGR





wet scavenging improved with inclusion of secondary activation

ice-borne aerosols had smaller effect (for this case)

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