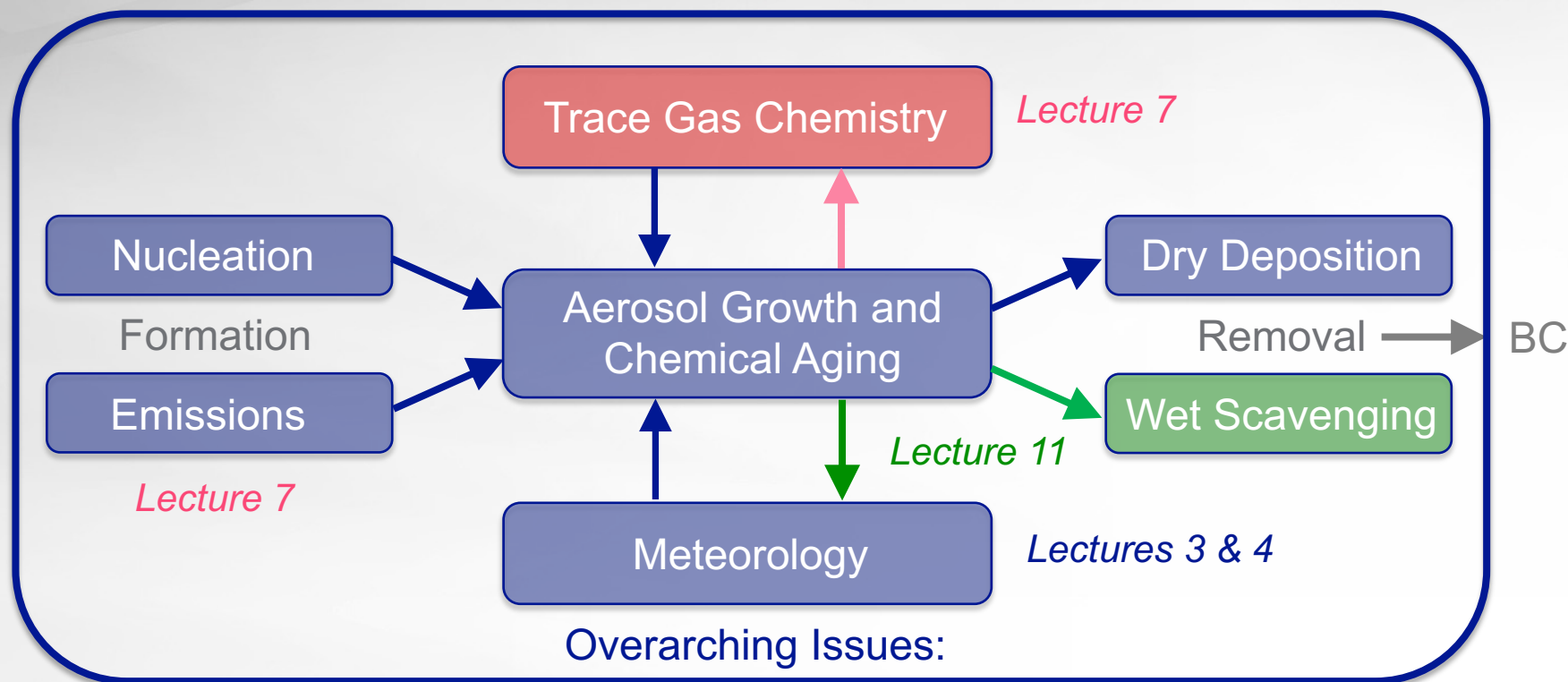


Modeling Aerosol Processes (all you need to know in 60 minutes or less)

JEROME FAST



Representation of Aerosol Size, Mixing State, and Morphology
Model Evaluation and Computational Expense

Lectures 1 & 2

Emission of Primary Particles and Gas-Phase Precursors

Natural Emissions

Sea Salt

- ▶ NaCl

Sea Spray

- ▶ DMS and organics

Dust

- ▶ inorganic minerals

Volcanic

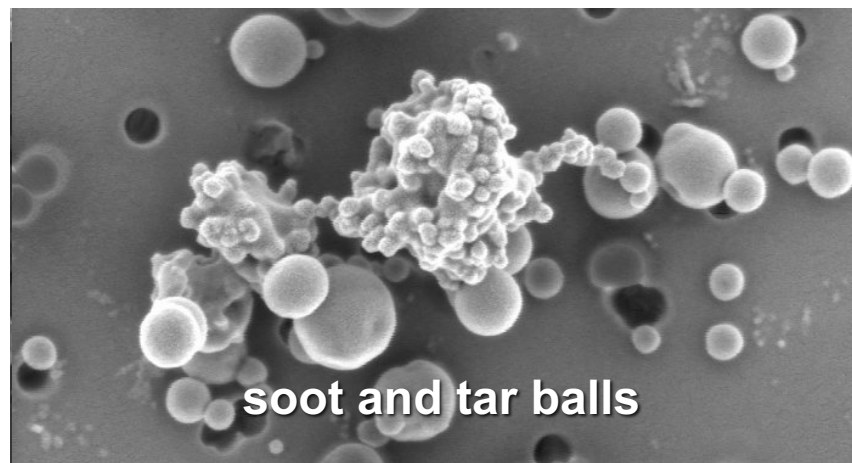
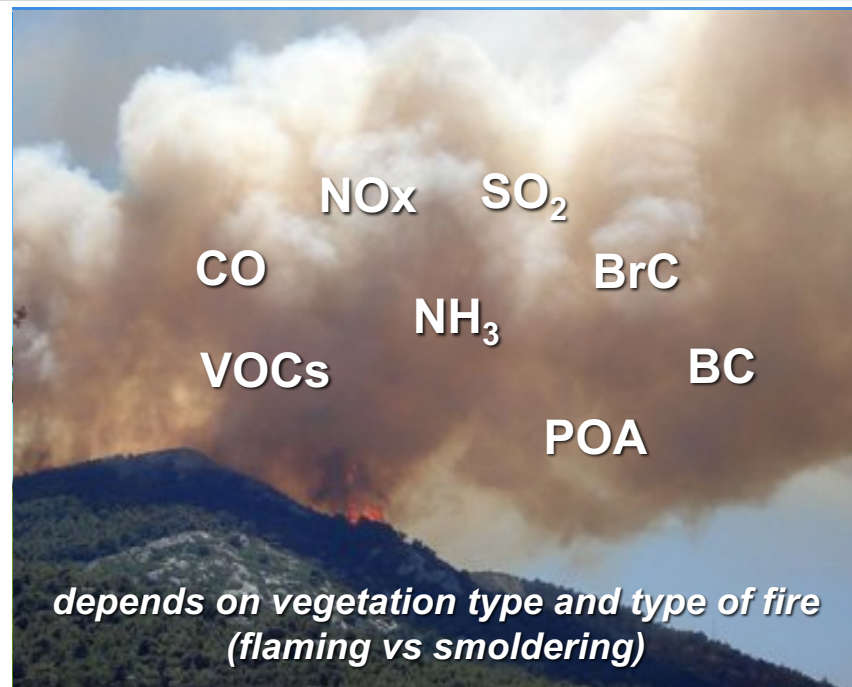
- ▶ fly ash
- ▶ SO₂ & other gases

Biogenic / Biological

- ▶ isoprene, monoterpenes, etc.
- ▶ spores, pollen, insect parts, etc.

Biomass Burning

- ▶ soot & primary organic aerosol (POA)
- ▶ VOCs & other gases

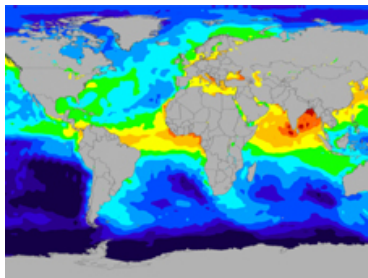


A Word About Dust Speciation ...



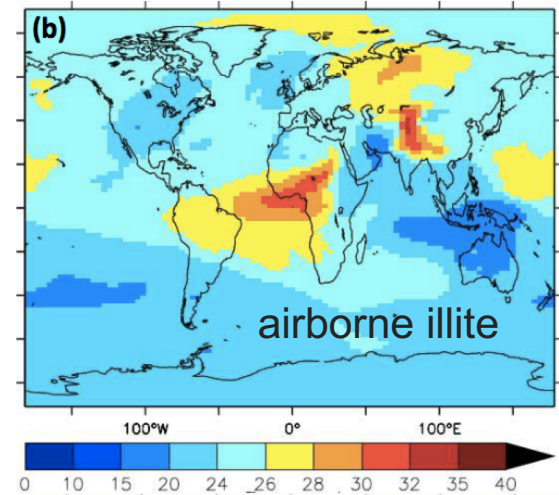
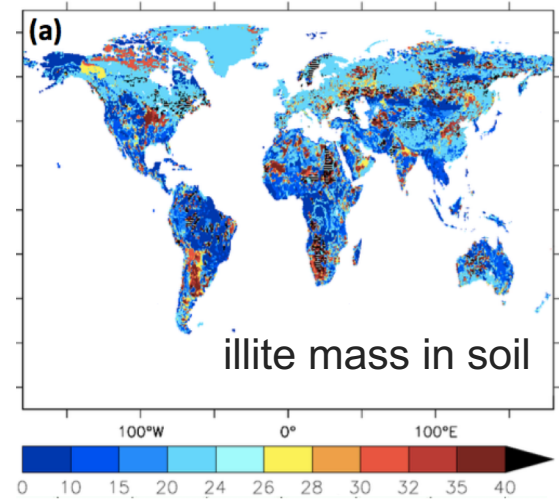
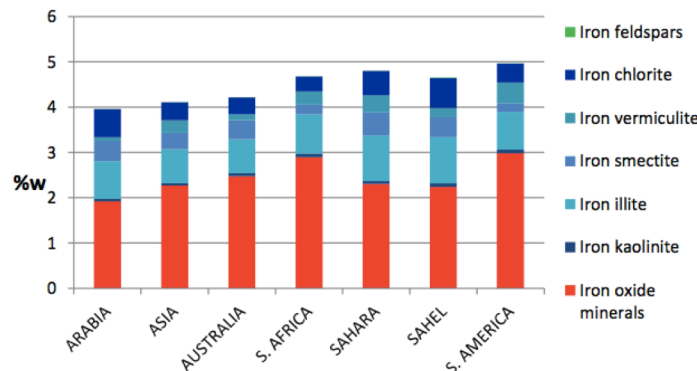
To Speciate or Not to Speciate ... That is the Question

- ▶ If one is interested only in the bulk effects of dust on concentration and radiative effects, then speciating dust is probably not important ...
- ▶ But, speciation into different minerals (illite, kaolinite, quartz, calcite, etc.) is important for:
 - Heterogeneous chemistry (e.g. CaCO_3 and HNO_3)
 - Complexity in treating ice nuclei (IN) 
 - Biogeochemical cycling of trace nutrients in climate models (ignored by air quality models)



iron deposition

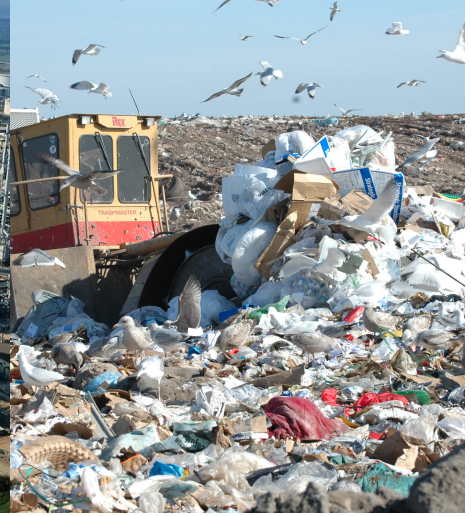
Iron Content in Soil by Region



from Journet et al. ACP, 2014

Anthropogenic Emissions: By Sector

Transportation



Waste

Energy Production



Industry



Agriculture

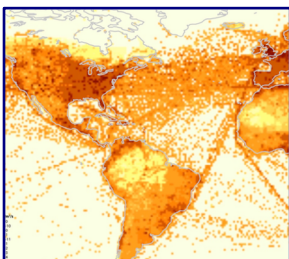


Other

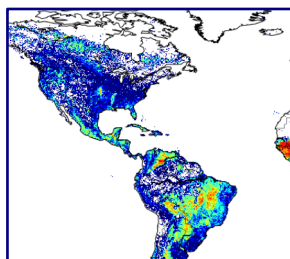


Representing Emissions in Models

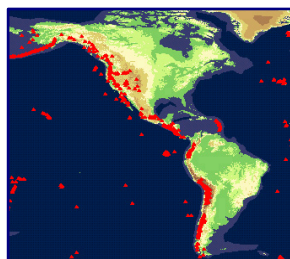
**Anthropogenic
Inventory**
point & area
sources



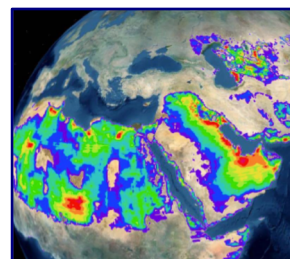
**Biomass Burning
Inventory**
point sources



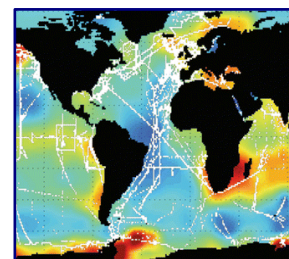
**Volcanic
Inventory**
point sources



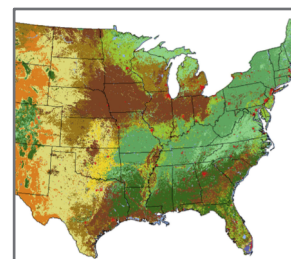
**Erodible Soil
Dataset**
area sources



**Oceanic
Biological
Dataset**
area sources



**Vegetation
Dataset**
area sources



Emission Processor

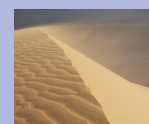
- ▶ **Reapportion** emission rates from native geographic information to model grid cells (conserve mass)
- ▶ **Merge** sector information
- ▶ **Map** trace gases and particulate species and convert units to be consistent with model mechanism
- ▶ **Assume** diurnal variation

**Emission
Files**

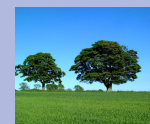
Model

online calculations of

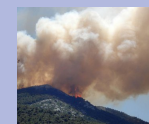
dust



biogenic



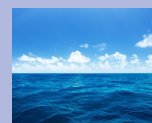
plume rise



sea-salt



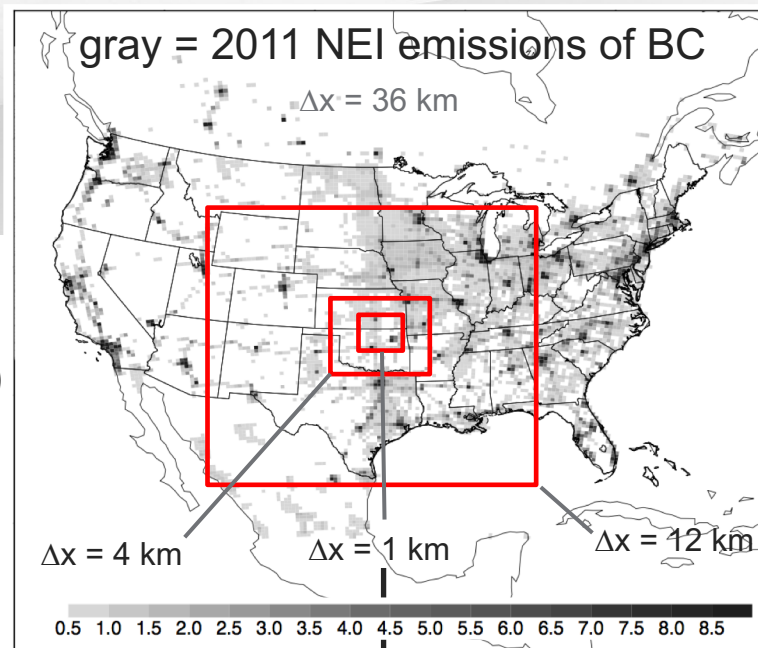
sea-spray



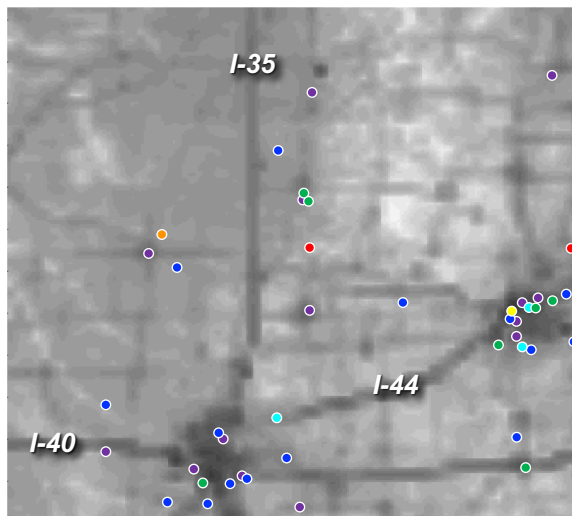
Emissions: Example

WRF-Chem Simulation

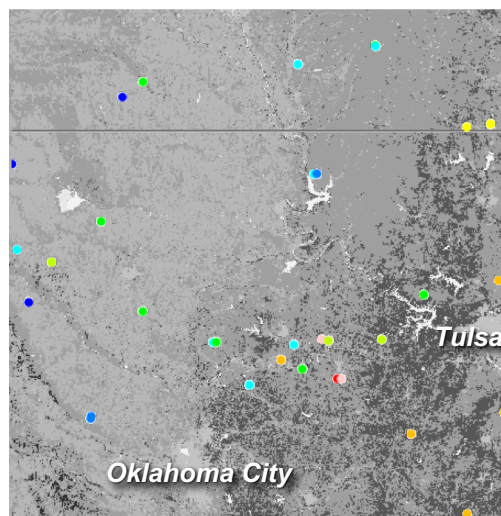
- ▶ 2011 National Emissions Inventory ($\Delta x = 4$ km)
- ▶ Fire INventory from NCAR (FINN)
- ▶ MEGAN biogenic emissions module



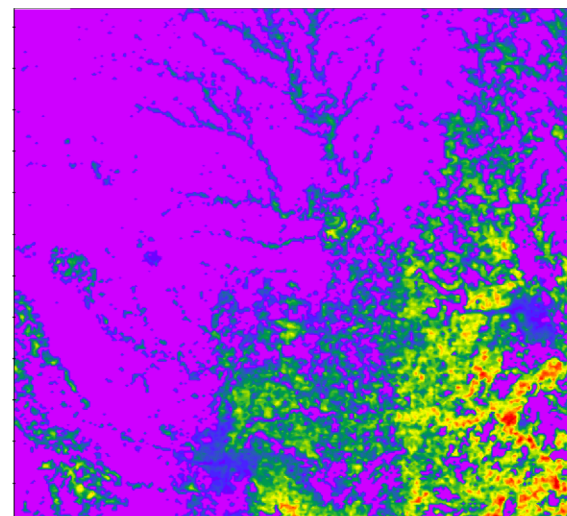
Anthropogenic:
BC (gray) & SO_2 (color)



Biomass Burning



Biogenic: Isoprene



New Particle Formation

Nucleation: New Particle Formation

Molecules and Small Clusters

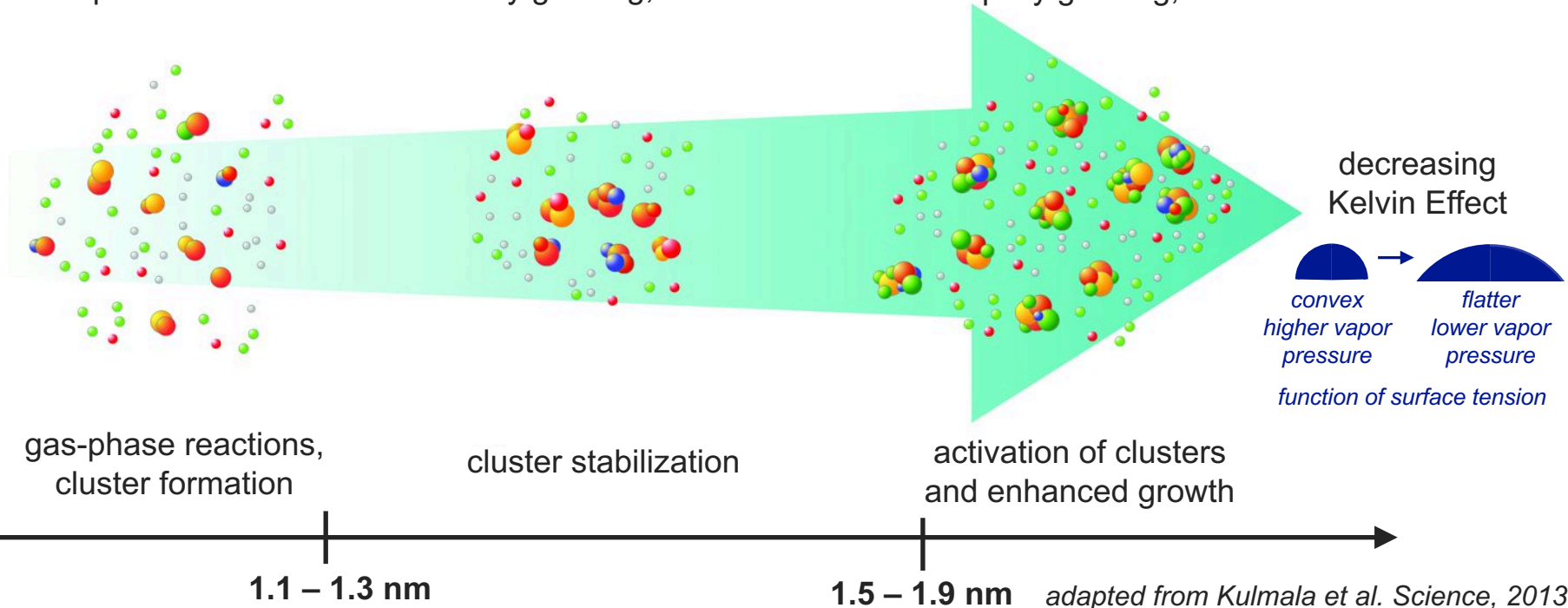
- Very slow growth
- Clusters form and evaporate

Critical Size for Clustering

- Sulfuric acid and amines
- Stabilizing organic compounds
- Slowly growing, $< 1 \text{ nm h}^{-1}$

Growing Clusters

- Organics start to dominate
- Nano-Kohler
- Rapidly growing, 2 nm h^{-1}

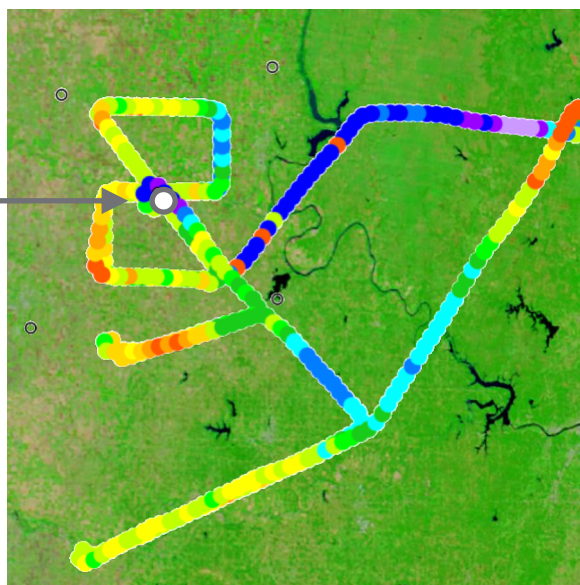
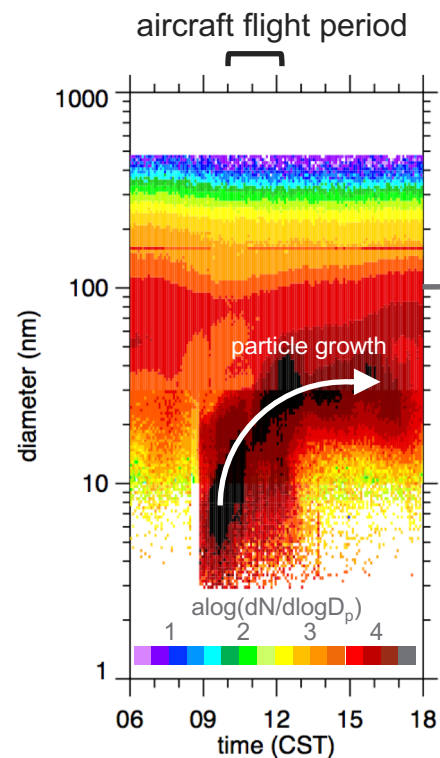


NPF tends to occur under “clean conditions” when concentrations of accumulation mode particles is relatively low, so that they do not compete for trace gases (sulfuric acid and organic compounds)

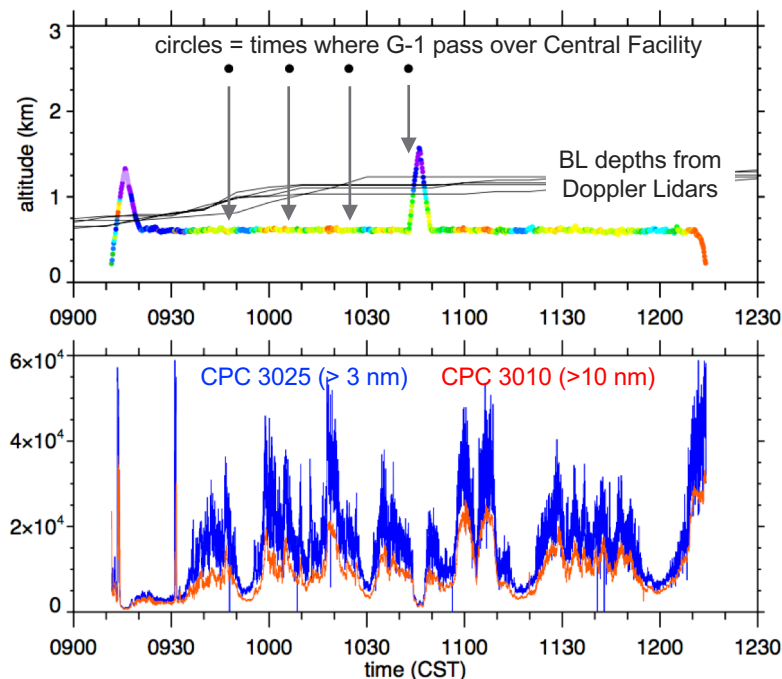
Nucleation: Observations

2016 HI-SCALE Field Campaign

North-Central Oklahoma



CPC 3025	> 36	18 - 24	8 - 10	2 - 4
(# cm ⁻³ * 10 ⁻³)	30 - 36	12 - 18	6 - 8	1 - 2
	24 - 30	10 - 12	4 - 5	< 1



from Fast et al., in review

- ▶ NPF events occurred frequently in the spring IOP, but were less frequent during the late summer IOP
- ▶ Few studies have characterized the observed spatial extent of NPF events

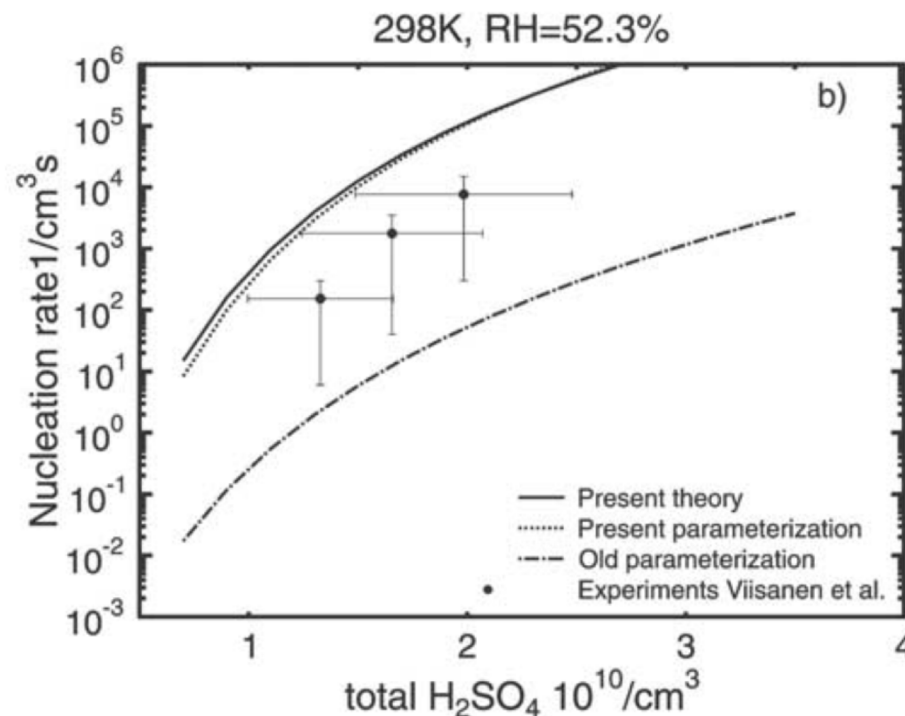
Nucleation: Parameterizations

Determine how many particles are formed based on ambient conditions, i.e. a formation rate J ($\# \text{ s}^{-1}$) or a growth rate (nm s^{-1}). Formation pathways likely different in the troposphere and stratosphere.

Empirical formulas based on theory and fits to observations:

- ▶ Binary homogeneous mechanism H_2SO_4 & H_2O
- ▶ Ternary nucleation mechanism H_2SO_4 , H_2O , and NH_3
- ▶ Ion-induced mechanism
- ▶ Combined organic and H_2SO_4 empirical mechanism

Model errors can easily be an order of magnitude or more, but ...



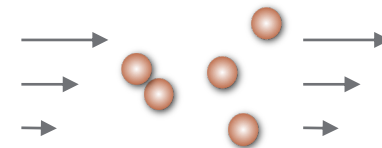
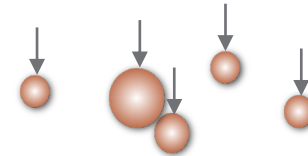
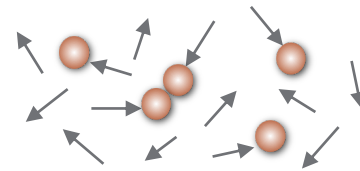
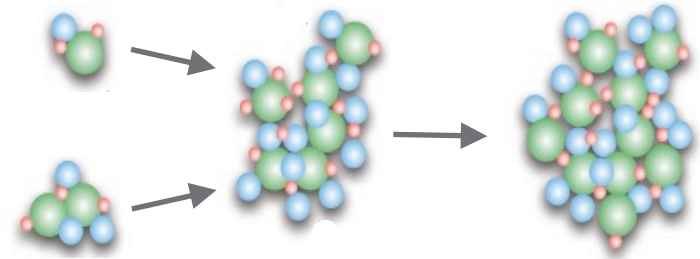
Aerosol Growth and Aging

Coagulation

Coagulation occurs when two particles collide and combine to form a larger particle.

Processes involved include:

- ▶ **Brownian motion:** Random collisions of particles that stick together
- ▶ **Gravitational Settling:** Particles that fall due to gravitational settling and then collide and stick to other particles. Settling velocities depend on particle size.
- ▶ **Turbulent Shear:** Motions induced by spatial turbulent fluctuations results in collisions of particle that stick together

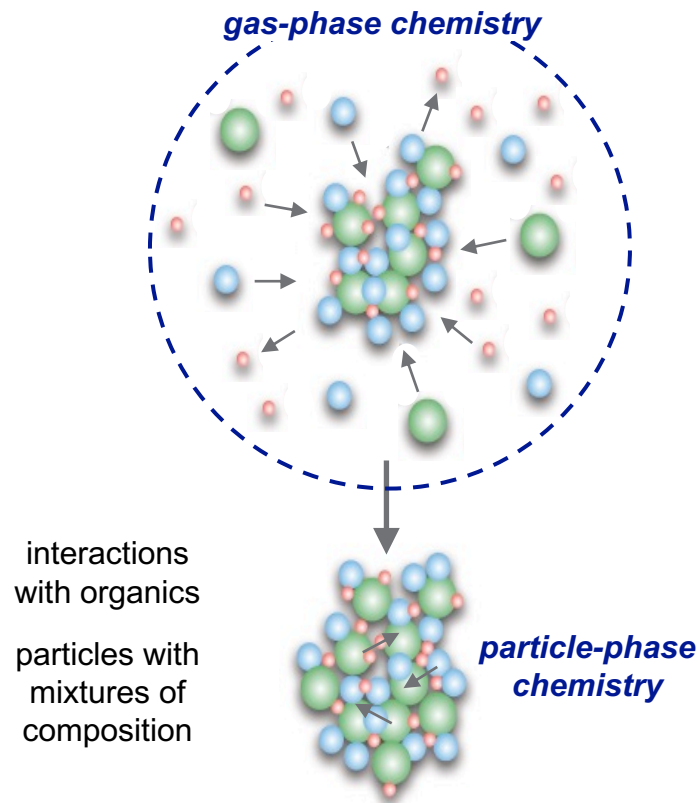


All enhanced by van der Waals forces (electrostatic attractive forces)

Condensation and Evaporation

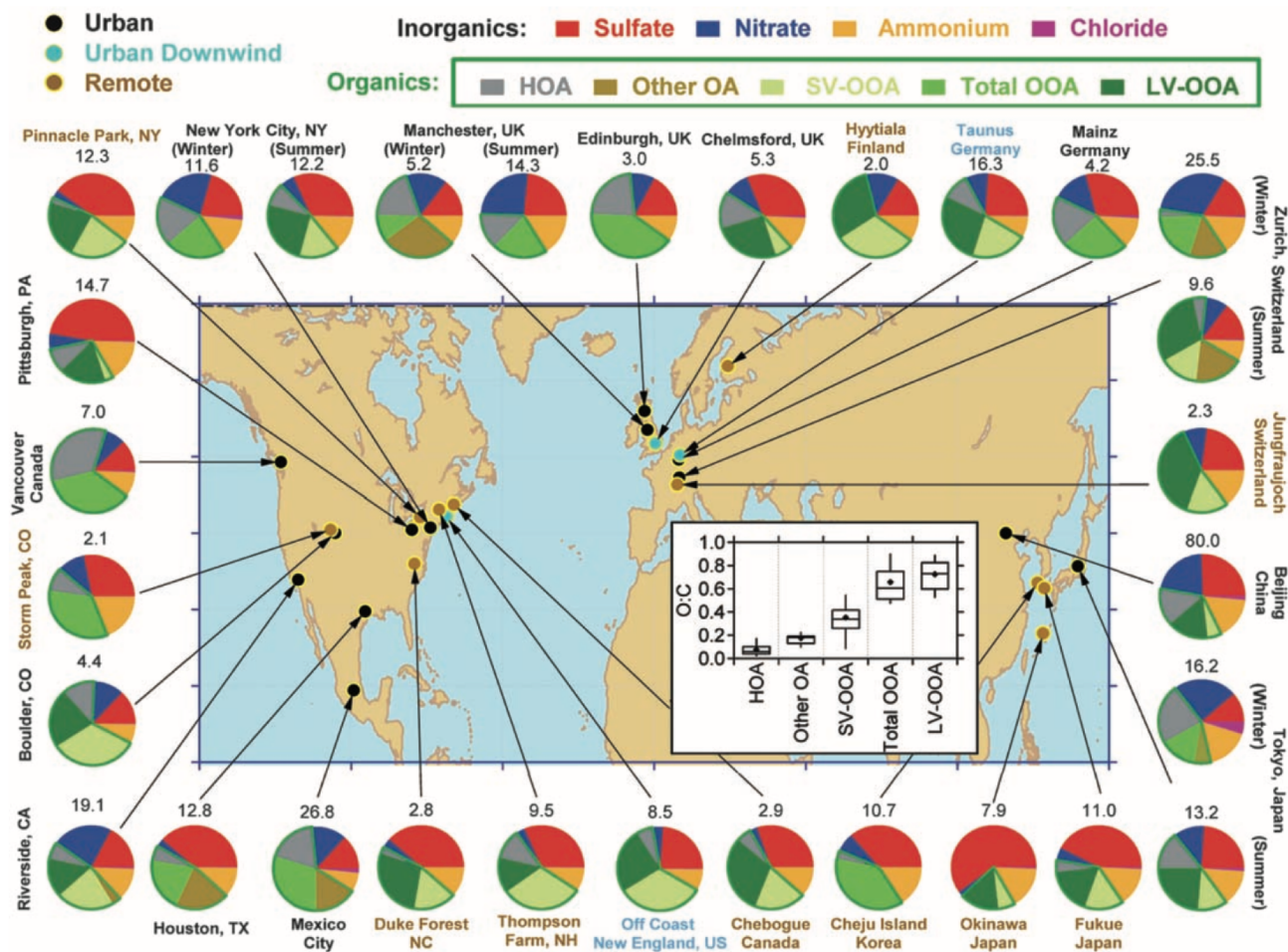
Condensations occurs when organic and inorganic trace gases condense on preexisting particles, forming secondary aerosol. Secondary aerosols include:

- ▶ **Sulfate, SO_4 :** oxidation of SO_2 by OH, aqueous chemistry
- ▶ **Nitrate, NO_3 :** oxidation of NO_2 by OH, aqueous chemistry
- ▶ **Ammonium, NH_4 :** $\text{NH}_3 + \text{HNO}_3$ forms NH_4NO_3 ; $\text{NH}_3 + \text{H}_2\text{SO}_4$ forms $(\text{NH}_4)_2\text{SO}_4$
- ▶ **Secondary Organic Aerosols (SOA):** many chemical pathways, many unknown



Observed Secondary Species

Aerosol Mass Spectrometers (AMS) are frequently used to characterize bulk composition for particle diameters $< 1 \mu\text{m}$:



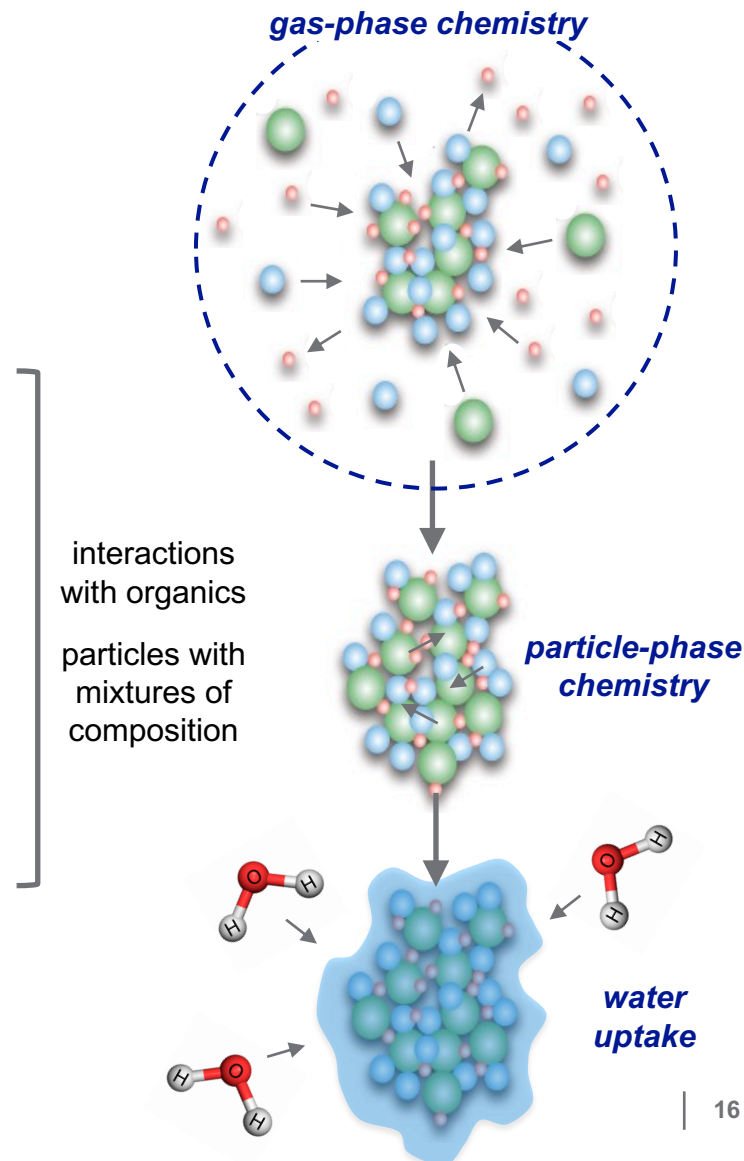
sulfate and organics dominate accumulation mode aerosol mass

Note: results depend on sampling period and season and most sampling sites located in or near urban areas

Condensation and Evaporation

Condensations occurs when organic and inorganic trace gases condense on preexisting particles, forming secondary aerosol. Secondary aerosols include:

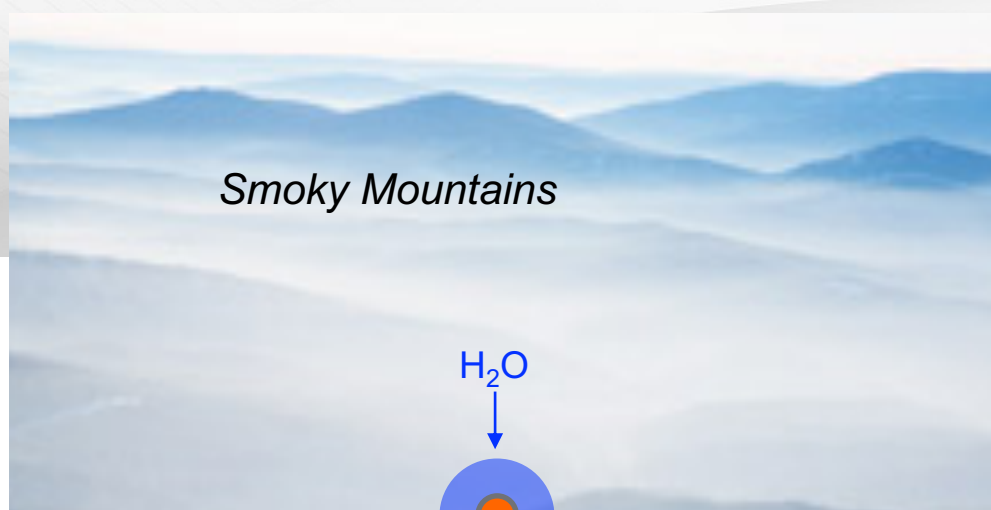
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- ▶ **Secondary Organic Aerosols (SOA):** many chemical pathways, many unknown
- ▶ **Water, H_2O :** depends on hygroscopic properties of pre-existing particle and RH



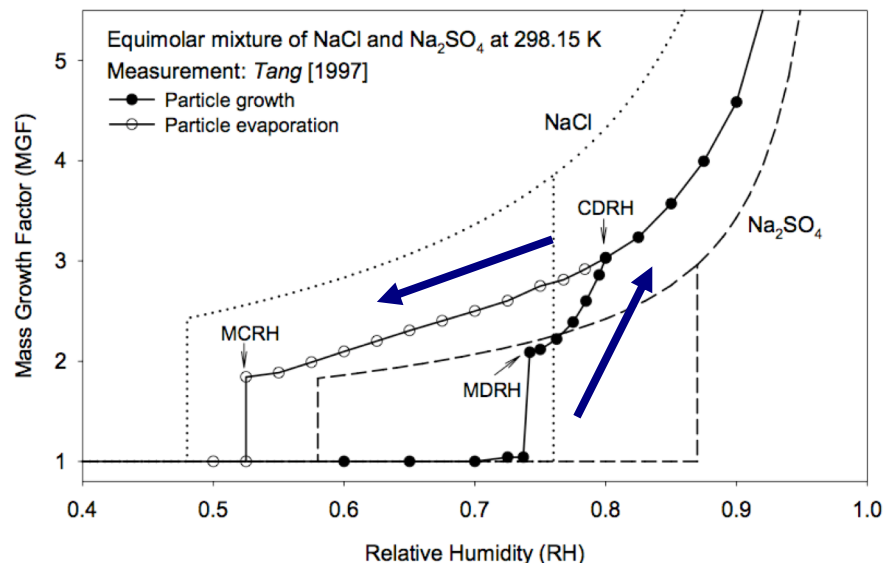
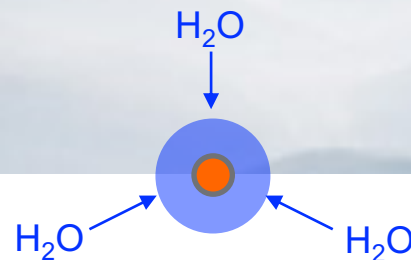
Hygroscopic Properties

Water uptake depends on aerosol composition (affinity to attract or repel water), aerosol size, and relative humidity (RH)

- ▶ SO_4 , NO_3 , NH_4 , and NaCl are hydrophilic, while OM and dust tend to be hydrophobic
- ▶ Petters and Kriedenweis, (2007) developed a single parameter, κ , to quantify hygroscopic growth potential; $0.1 < \kappa < 0.9$
- ▶ Hysteresis effect important in determining aerosol water when ambient RH changes
- ▶ Water uptake important for aqueous phase chemistry. It also significantly affects aerosol optical properties (more scattering) and contribute a large fraction of observed AOD.

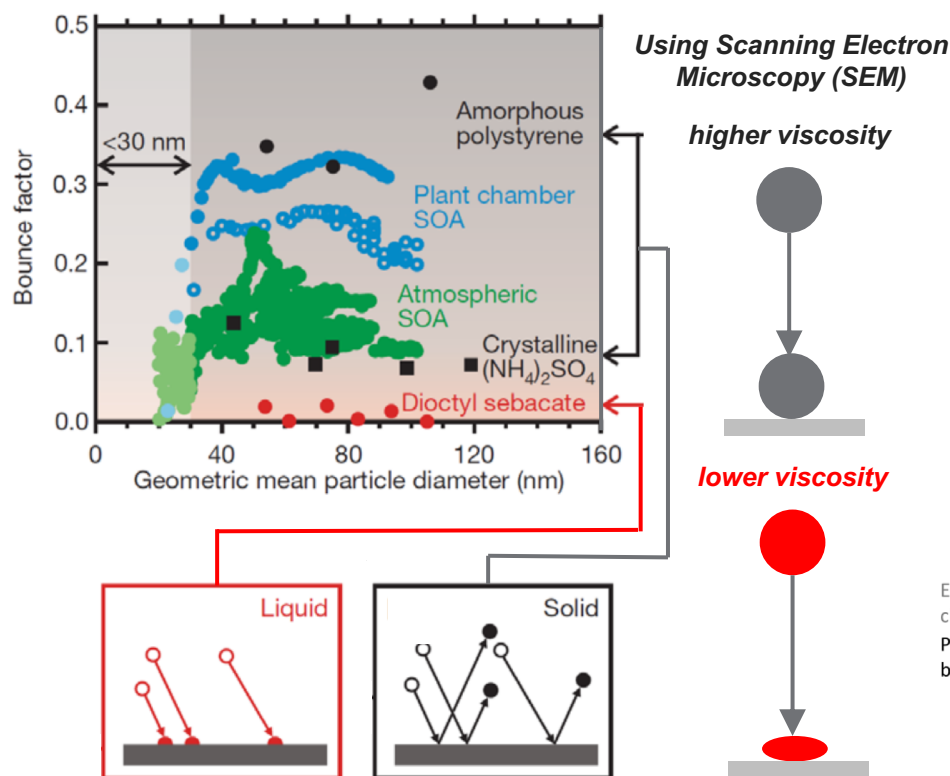


Smoky Mountains

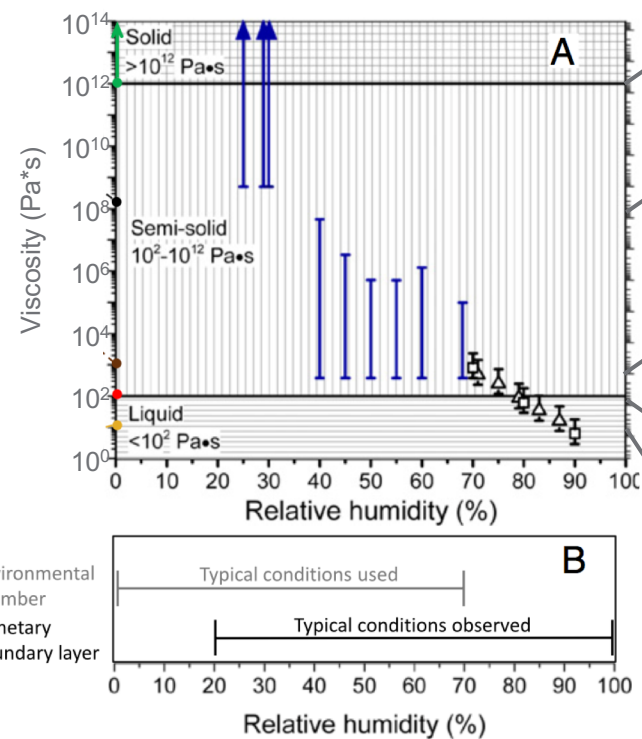


OA Properties in a Nutshell (1)

- ▶ Phase and volatility affect condensation and evaporation
- ▶ Organic matter (OM) used to be thought of as a liquid and simulated by using an equilibrium approach. Over the past decade, new observational techniques show that OM can be liquid, semi-solid, or solid depending on the specific organic compounds and environmental conditions (temperature and RH).



from Virtanen et al., 2010



from Renbraum-Wolff et al. PNAS, 2013

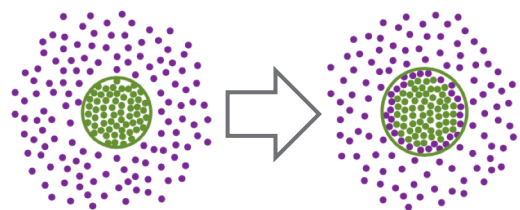
OA Properties in a Nutshell (2)

- Phase and volatility affects rate of chemical reactions and composition. Viscosity affects how deeply material penetrates or whether that material can escape from a particle.

OM Growth Mechanism and Rate

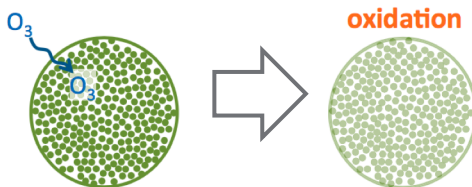


low viscosity particle

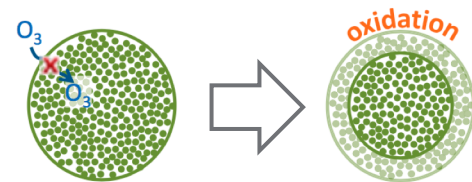


high viscosity particle

Heterogeneous Oxidation by O_3

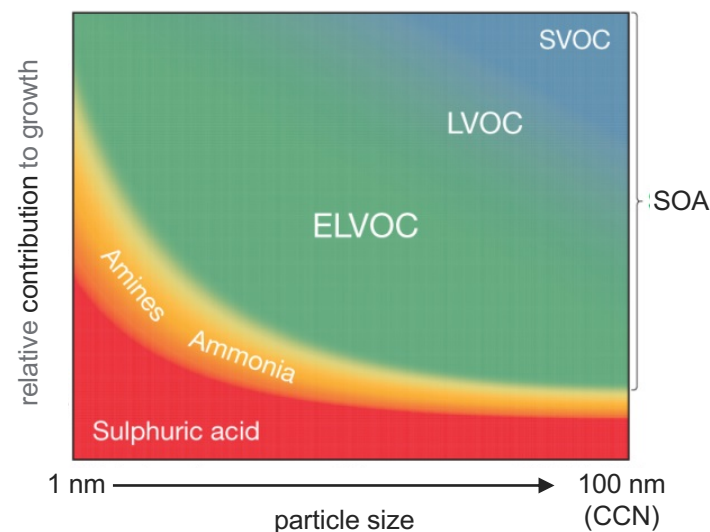


low viscosity particle



high viscosity particle

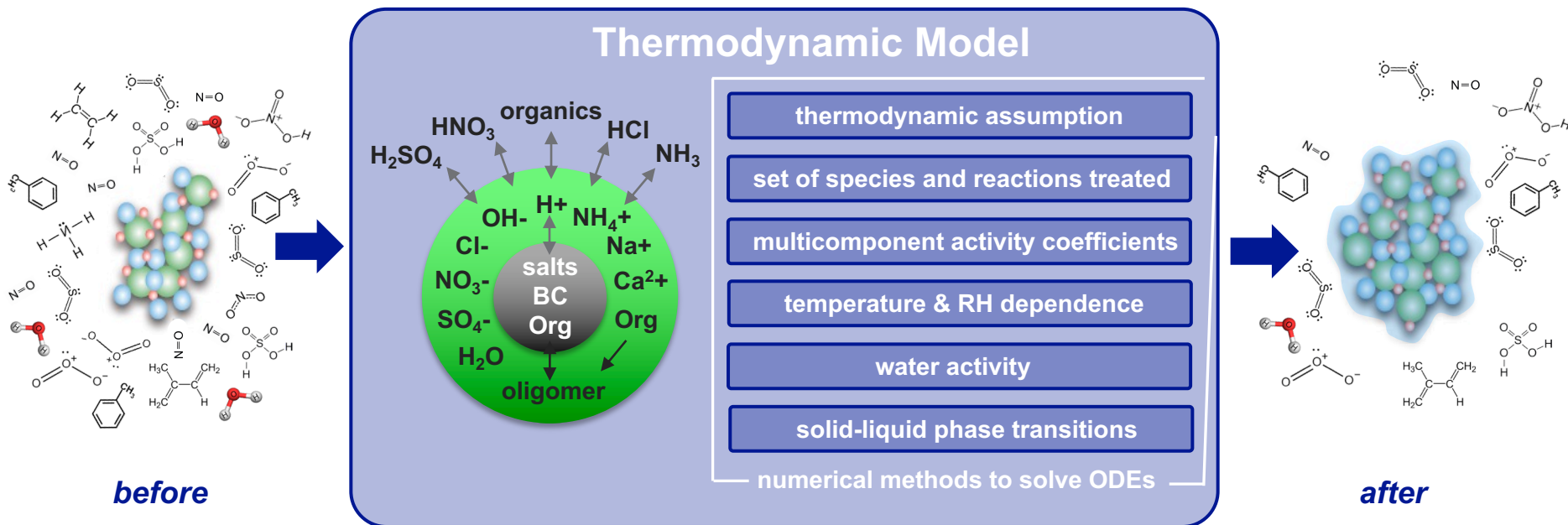
from Renbraum-Wolff et al. PNAS, 2013



from Ehn et al. Nature, 2014

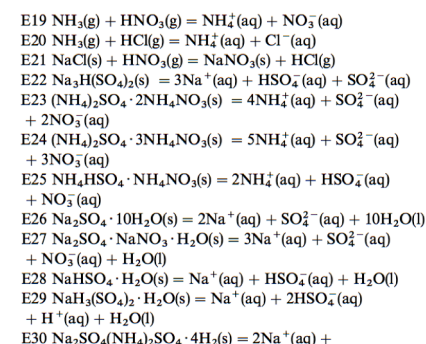
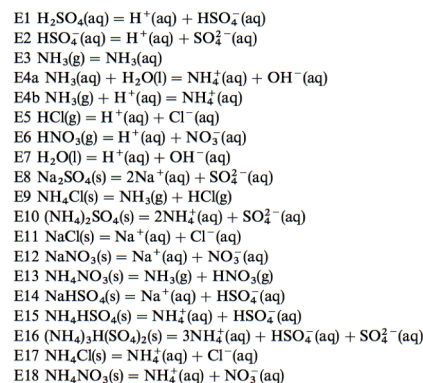
- SOA chemistry and properties are complex; therefore, the number of precursors and types of OM makes the understanding and modeling SOA challenging.

Modeling Gas-to-Particle Partitioning (1)



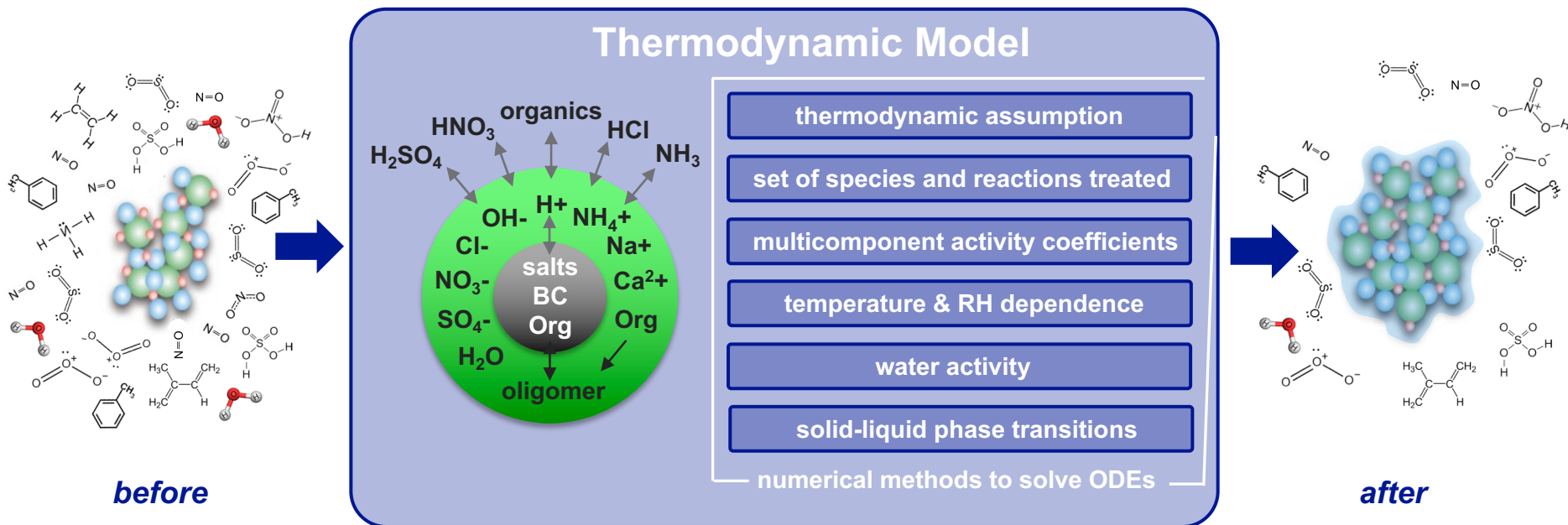
Model complexity varies greatly due to # of species and reactions treated, and assumptions

- **Equilibrium:** Assumes that volatile species in the gas and particle phase are in equilibrium.
- **Dynamic:** Observational and theoretical studies demonstrate that equilibrium assumption is not always valid for typical atmospheric conditions.
- **Hybrid:** Combination of equilibrium & dynamic



+ lots more ...

Modeling Gas-to-Particle Partitioning (1)



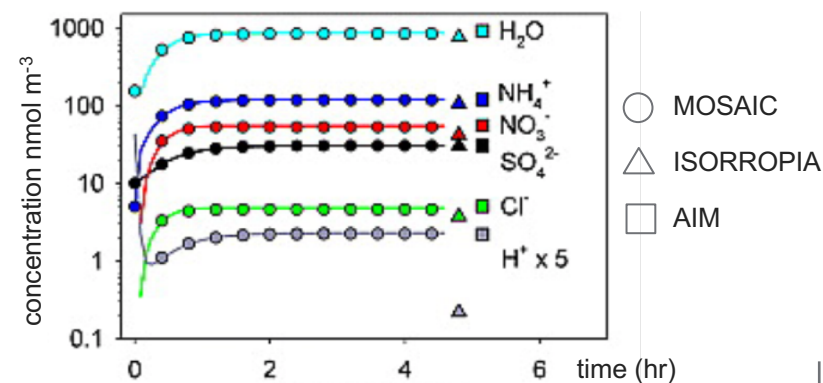
Many thermodynamic models have been developed since the 1980's, some suitable for box models and others suitable for use in 3-D atmospheric models

SCAPE **MOSAIC**

MARS **ISORROPIA** **E-AIM**

SEQUIBLIB **AIOMFAC** **EQUISOLV**

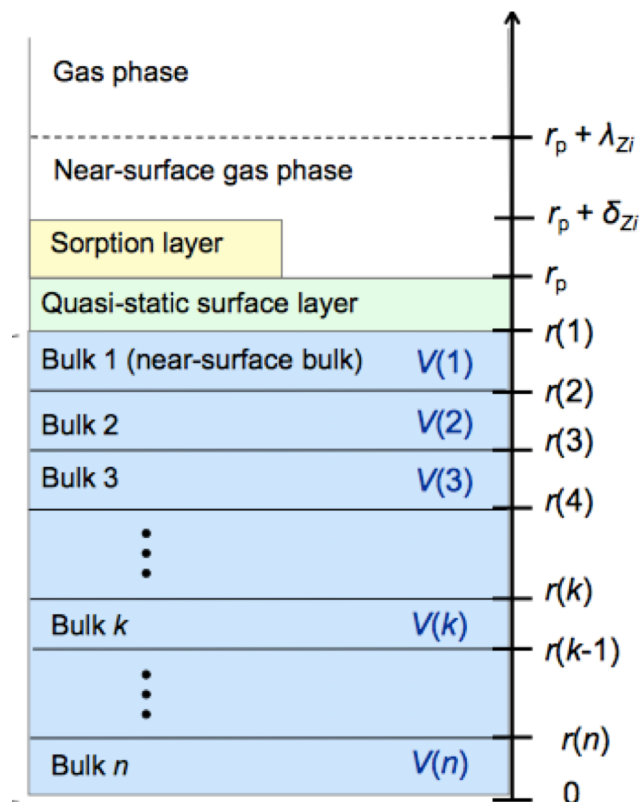
Evaluated using theory and/or laboratory data



Modeling Gas-to-Particle Partitioning (2)

Recent laboratory and field findings leading to more complex treatments of gas-to-particle partitioning.

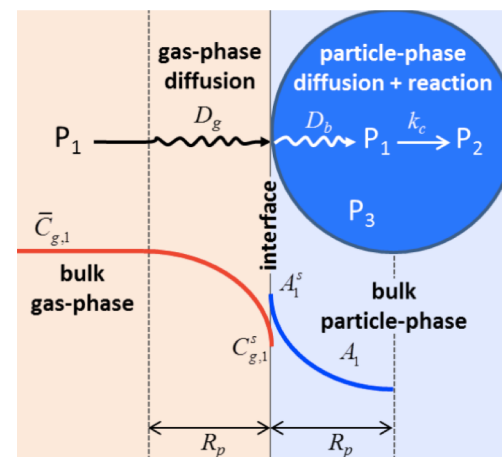
Kinetic Multi-Layer of Gas-Particle Interactions in Aerosols and Clouds (KM-GAP)



from Shiraiwa et al. ACP, 2012

treats all steps of mass transport and chemical reaction from the gas phase to the particle core, including semi-volatile species

New Version of MOSAIC



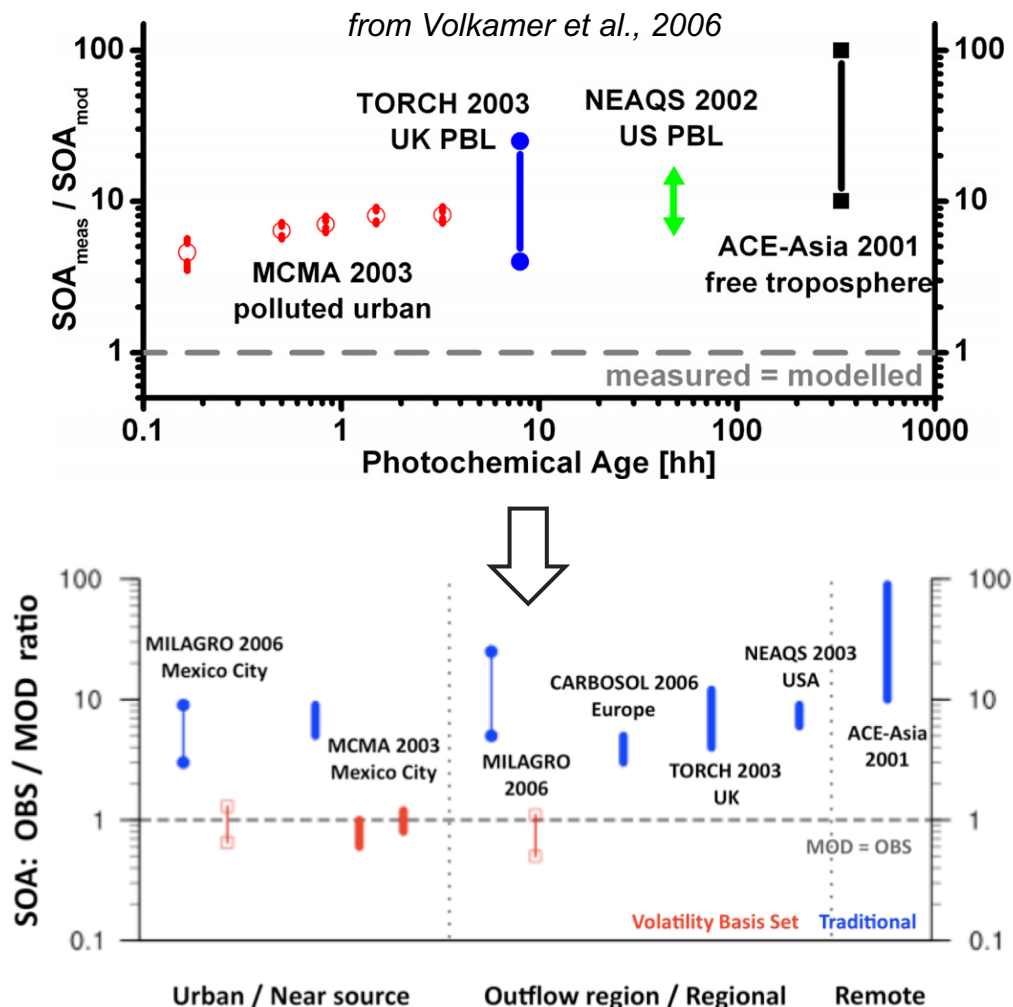
from Zaveri et al. ACP, 2014

Uses an analytical quasi-steady-state treatment for the diffusion-reaction process within the particle phase for fast-reacting organic solutes, and a two-film theory approach for slow- and non-reacting solute.

Modeling Gas-to-Particle Partitioning of Organics (1)

- ▶ Most 3-D models used to rely on semi-empirical parameterizations of chamber experiments to predict SOA mass
- ▶ Progress has been made in predicting SOA mass using more complex treatments, though it is still challenging
- ▶ Next step is to *simultaneously* predict more detailed extensive (number-size distributions) and intensive (O:C, viscosity) properties

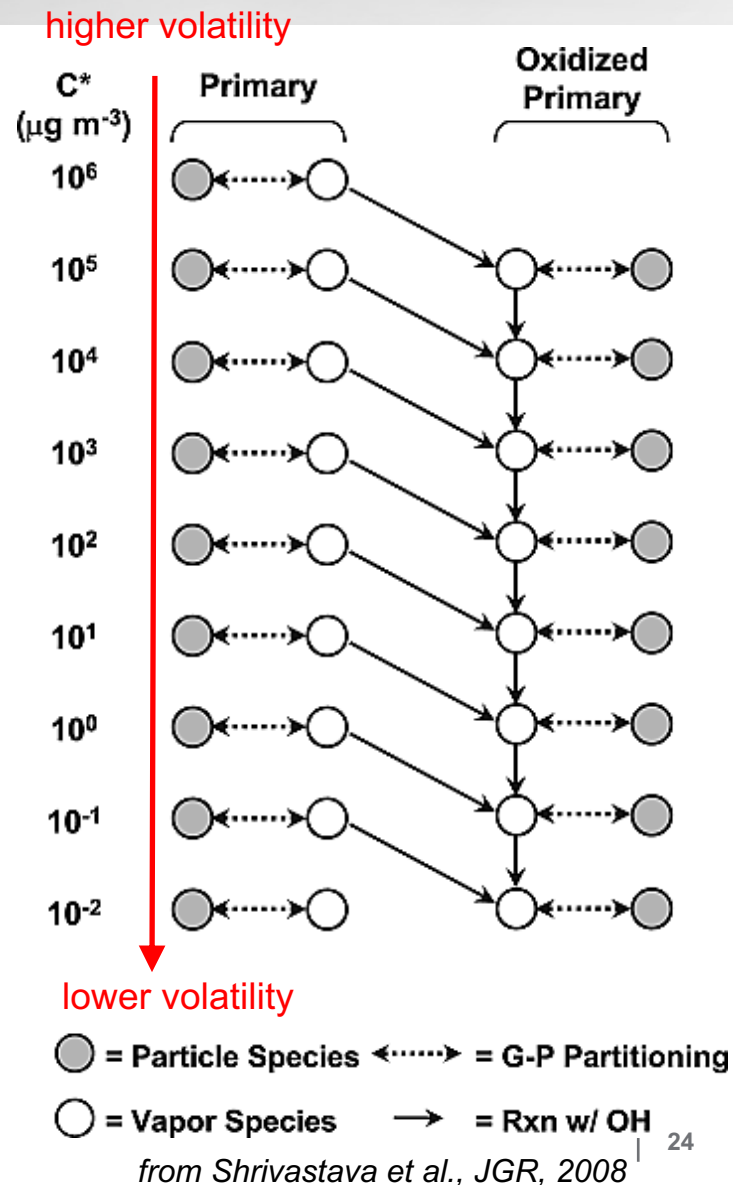
Note: Knowledge of organics changes rapidly. Published information can be out-of-date in a matter of months.



from Hodzic et al. ACP, 2010

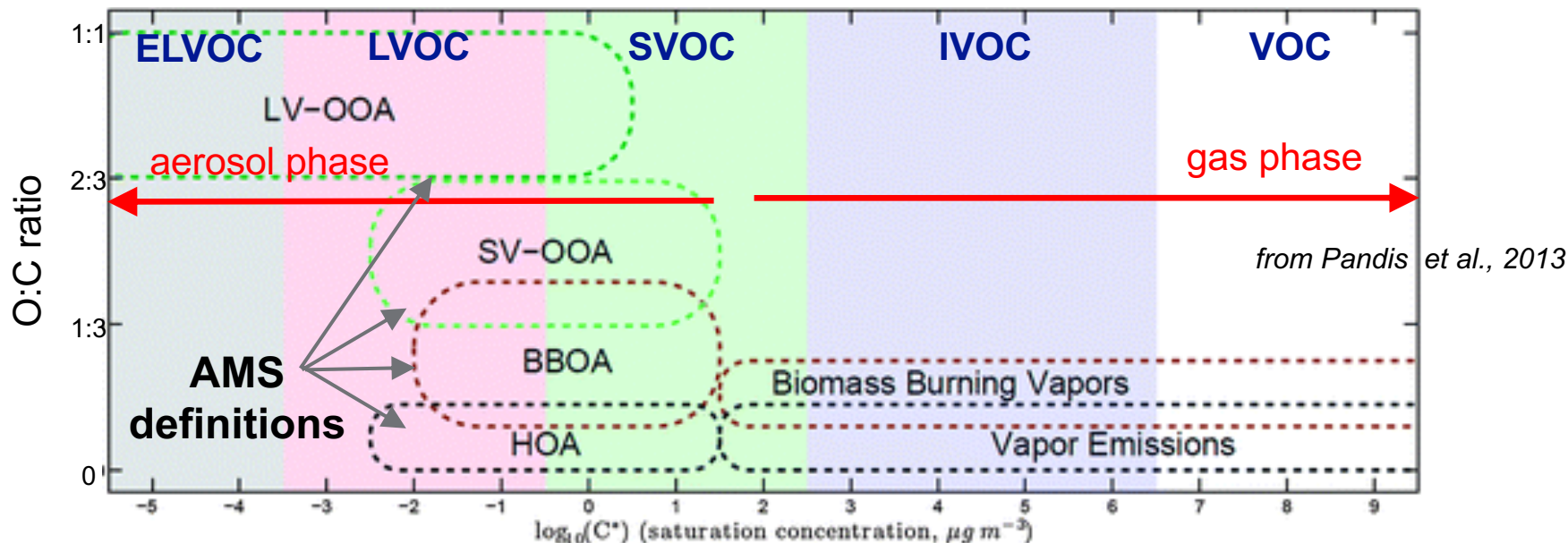
Modeling Gas-to-Particle Partitioning of Organics (2)

- ▶ Versions of the **Volatility Basis Set (VBS)**, see Robinson et al. 2007) approach now widely used to simulate SOA. Instead of explicitly simulating all of the reactions associated with the formation and evaporation of SOA (which is still incomplete), lump organics into a **discrete number of bins** based on their saturation concentration, C^* .
- ▶ Assumes that a series of oxidation reactions, that add an amount of oxygen per generation, will effectively move more and more aerosol mass into lower volatility bins.
- ▶ Volatility distributions are defined by fitting partitioning theory to experimental data. VBS models **vary significantly** depending on the number of bins used, the particular datasets used to constrain the model, assumed parameters, etc.



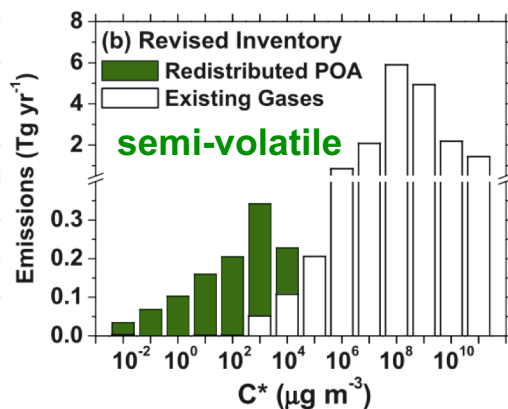
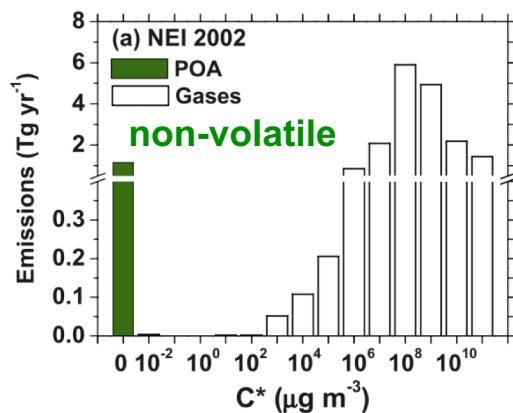
Modeling Gas-to-Particle Partitioning of Organics (3)

Sources and Processing of Organics



Treating POA Emissions

from Shrivastava et al. JGR, 2008



Biomass Burning and SOA



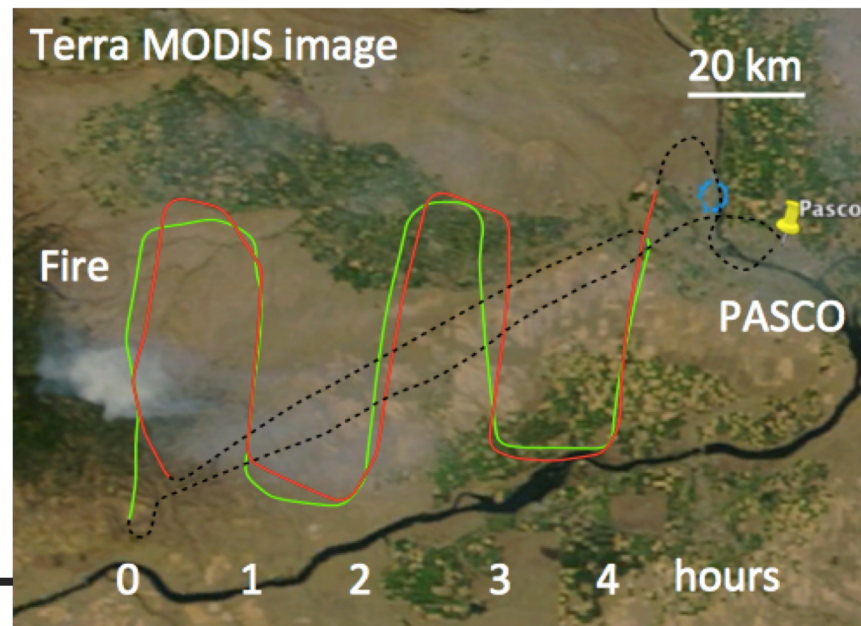
Do fires produce SOA? Some observational studies show that some fires produce SOA, while others do not possibly due to:

- ▶ Differences in fuel type
- ▶ Fire conditions (flaming vs smoldering)
- ▶ Dilution
- ▶ Limitations of laboratory (wall losses) or field data (sampling strategy)

Therefore, how SOA is represented in models is a **controversial subject**.

“Different approaches to the calculation of OA enhancement in ambient plumes can lead to different conclusions regarding SOA formation” (Bian et al. ACP, 2017)

DOE BBOP Campaign, 2013



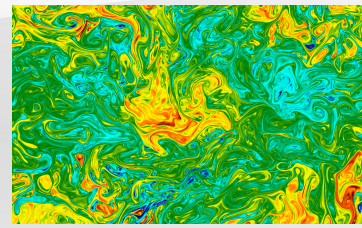
dilution decreases OA concentrations

concentration increases due to SOA

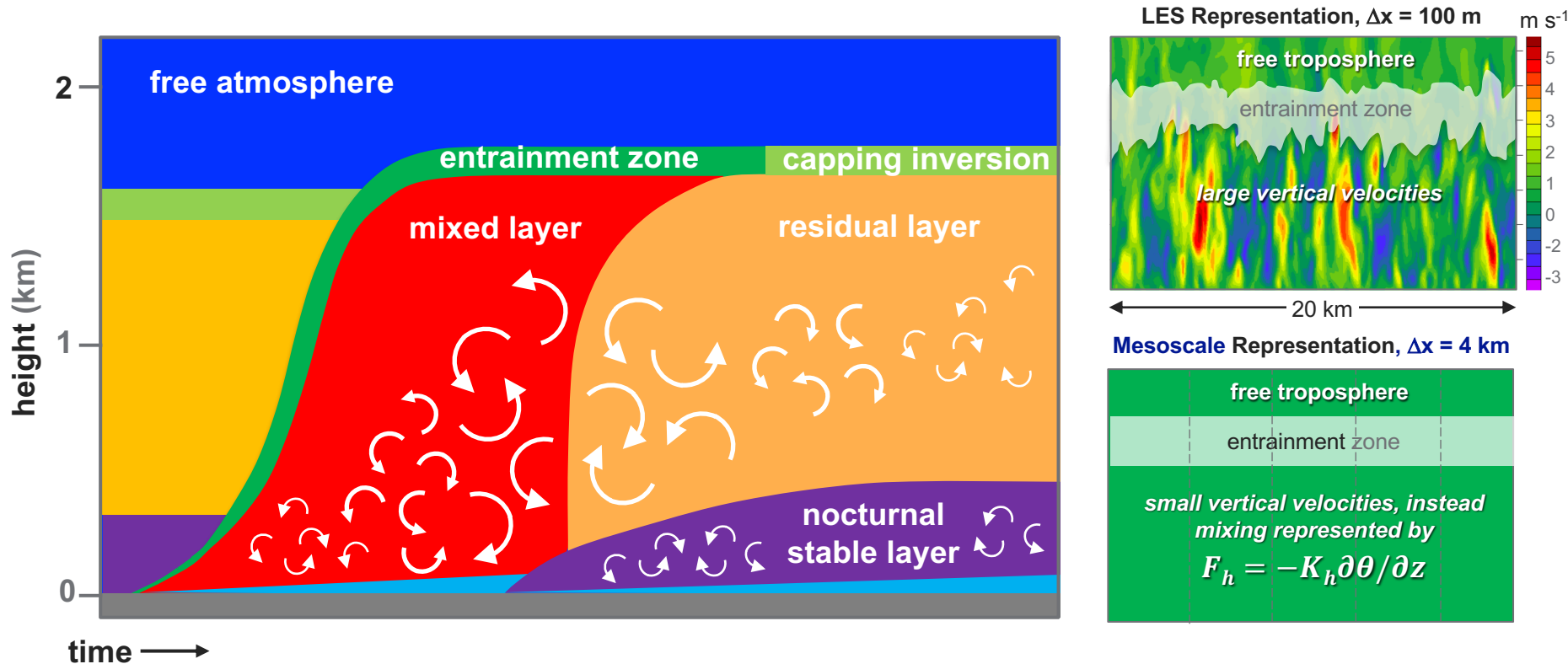


**and now, time for some meteorology that
affects aerosol distributions and gas-to-
particle partitioning ...**

The Role of Turbulent Mixing



- Turbulent motions near the Earth's surface vertically transport trace gases and aerosols, thereby diluting surface concentrations. In contrast, the growing daytime mixed layer will entrain tracers from the free troposphere to the surface.



- Mesoscale models rely on boundary-layer parameterizations to represent the overall effect of the subgrid-scale motions on atmospheric tracers. Model uncertainties are larger in the nocturnal stable layer and free troposphere.

The Role of Multi-scale Circulations

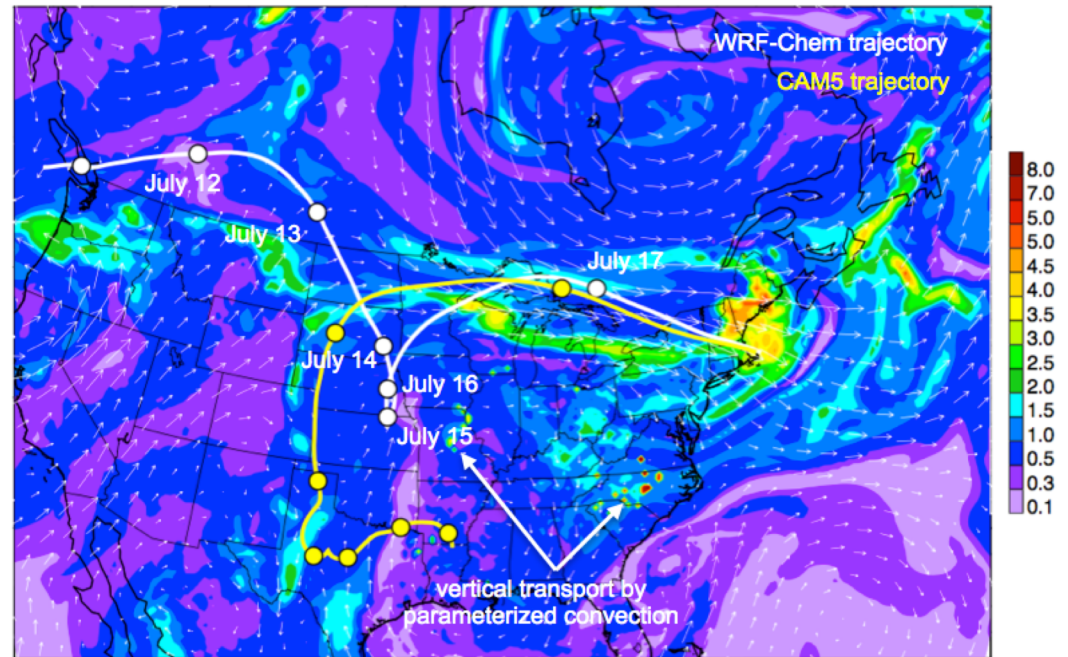
- ▶ Multi-scale circulations transport trace gases and aerosols over large distances
- ▶ Mesoscale models resolve many types of circulations, but global models with their coarser resolution poorly resolve or cannot resolve many circulations



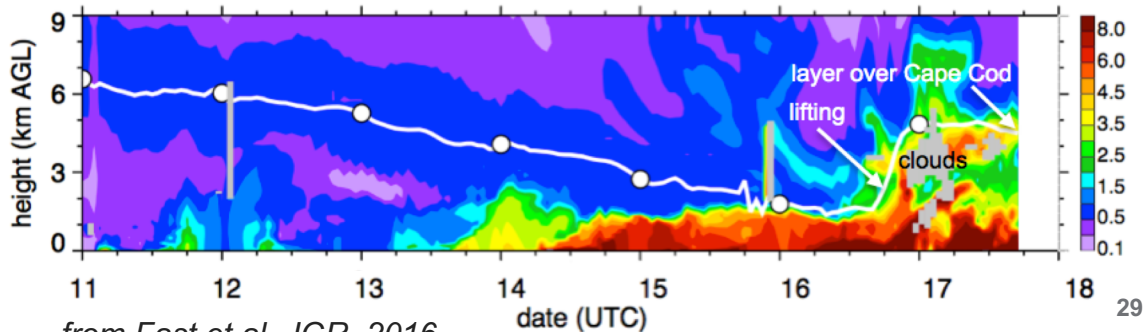
*regionally-refined grids
will only help so much*

Aerosol Layers Observed During TCAP Campaign

(a) WRF-Chem PM2.5 ($\mu\text{g m}^{-3}$) ~ 4.5 km AGL at 17 UTC, 17 July 2012



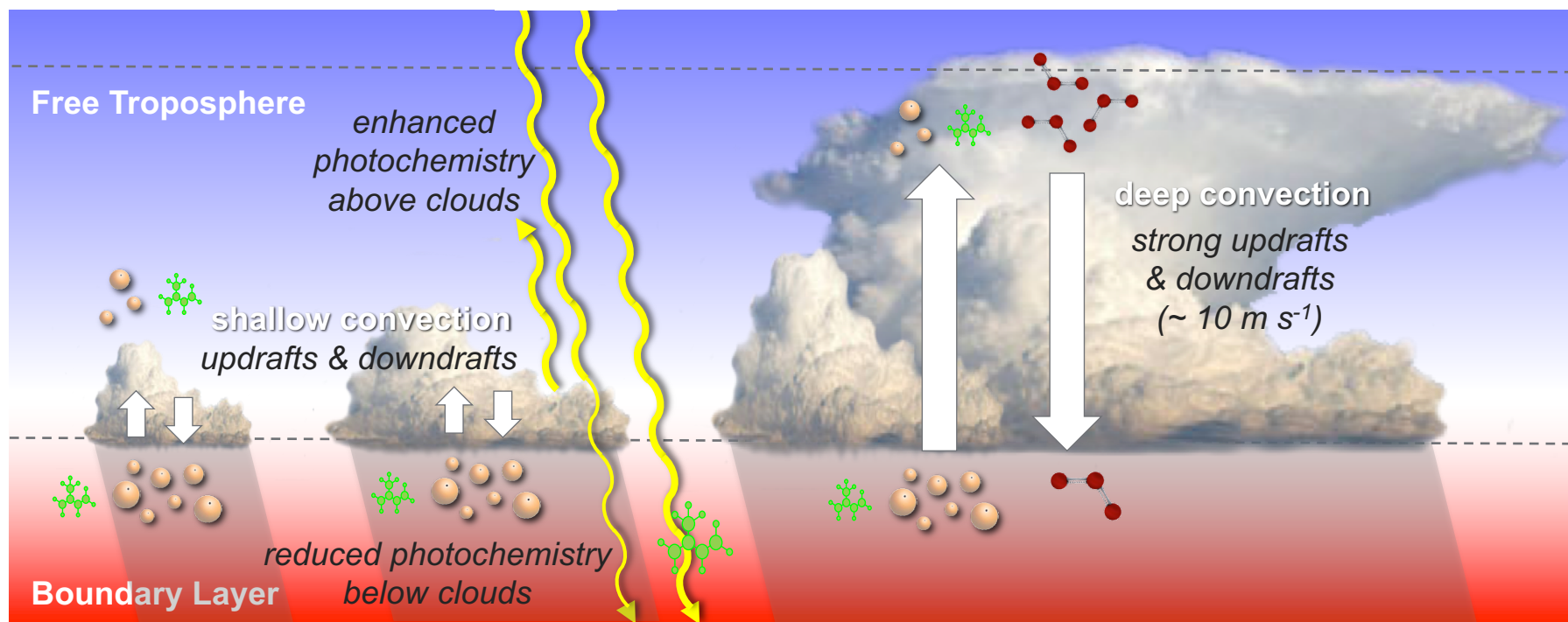
(b) WRF-Chem PM2.5 ($\mu\text{g m}^{-3}$) along white back trajectory in (a)



from Fast et al. JGR, 2016

The Role of Clouds

- ▶ Updrafts and downdrafts within clouds transport aerosols vertically more rapidly than mean ambient motions

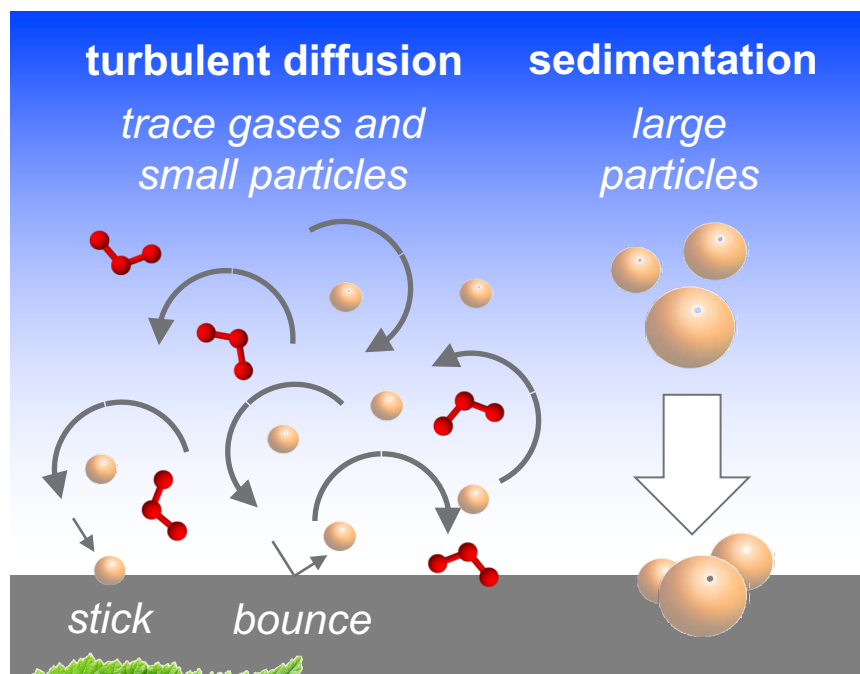


- ▶ Updrafts & downdrafts explicitly represented by “cloud-resolving” simulations, but vertical transport represented by convective parameterizations for $\Delta x \sim 10 \text{ km}$
- ▶ Simulations of clouds have relatively large uncertainties that will impact simulated trace gas and aerosol distributions

**and meteorology also affects removal of
aerosols from the atmosphere ...**

Dry Deposition

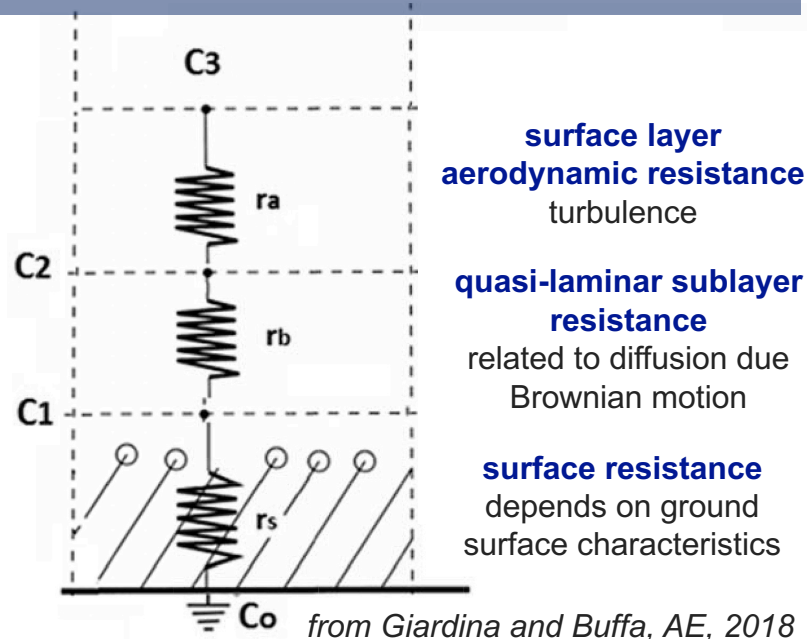
Dry deposition is a process that remove trace gases and particulates from the atmosphere and deposits them to the surface



rate depends on
particle size

rate depends on
type of surface

models often parameterize turbulent diffusion pathway using an electrical analogy (Wesely et al. 1995)

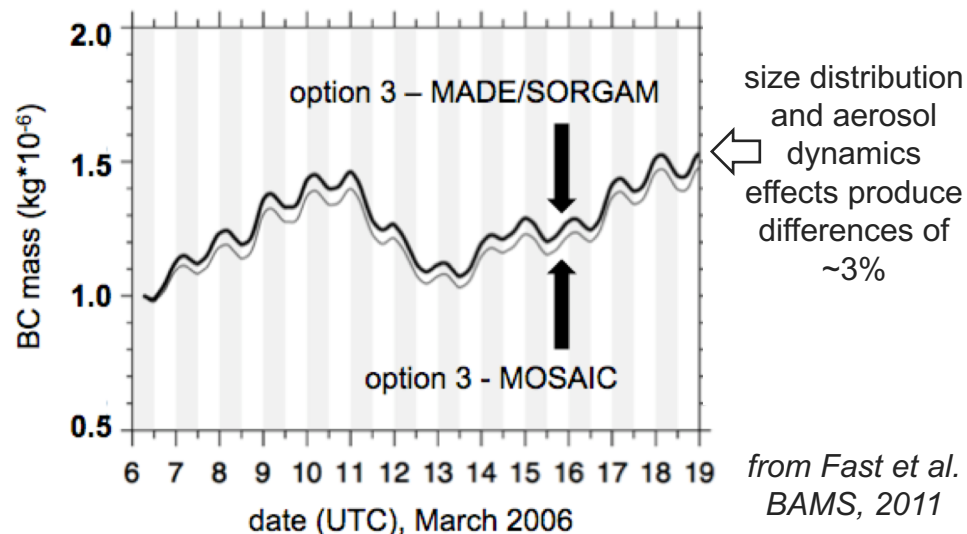
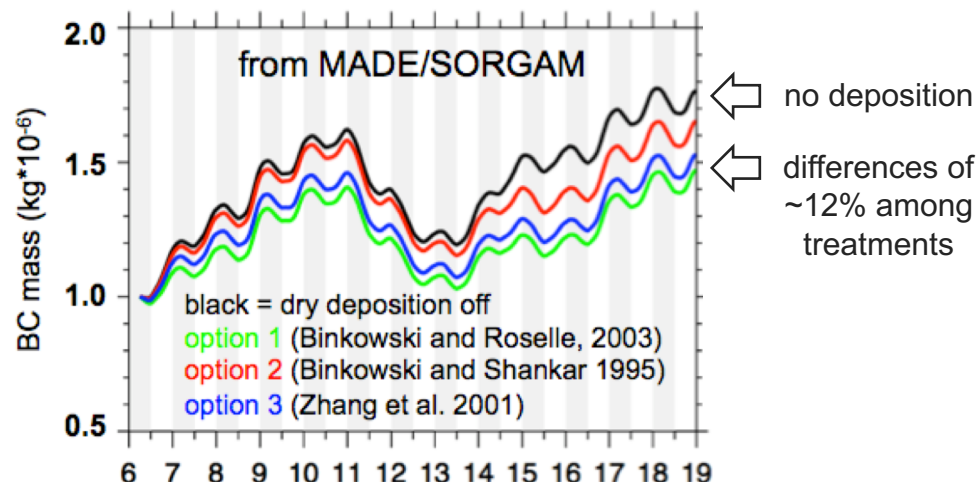


largest unknowns are removal rates
of SOA precursor gases

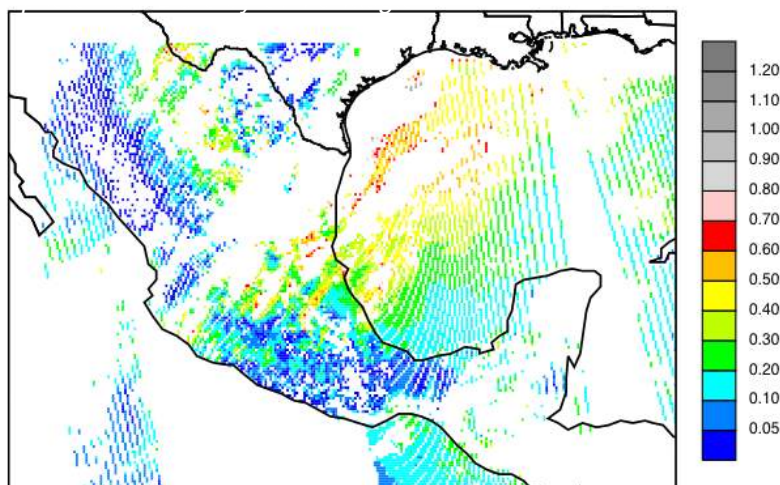
Impact of Dry Deposition



Simulated Black Carbon Mass

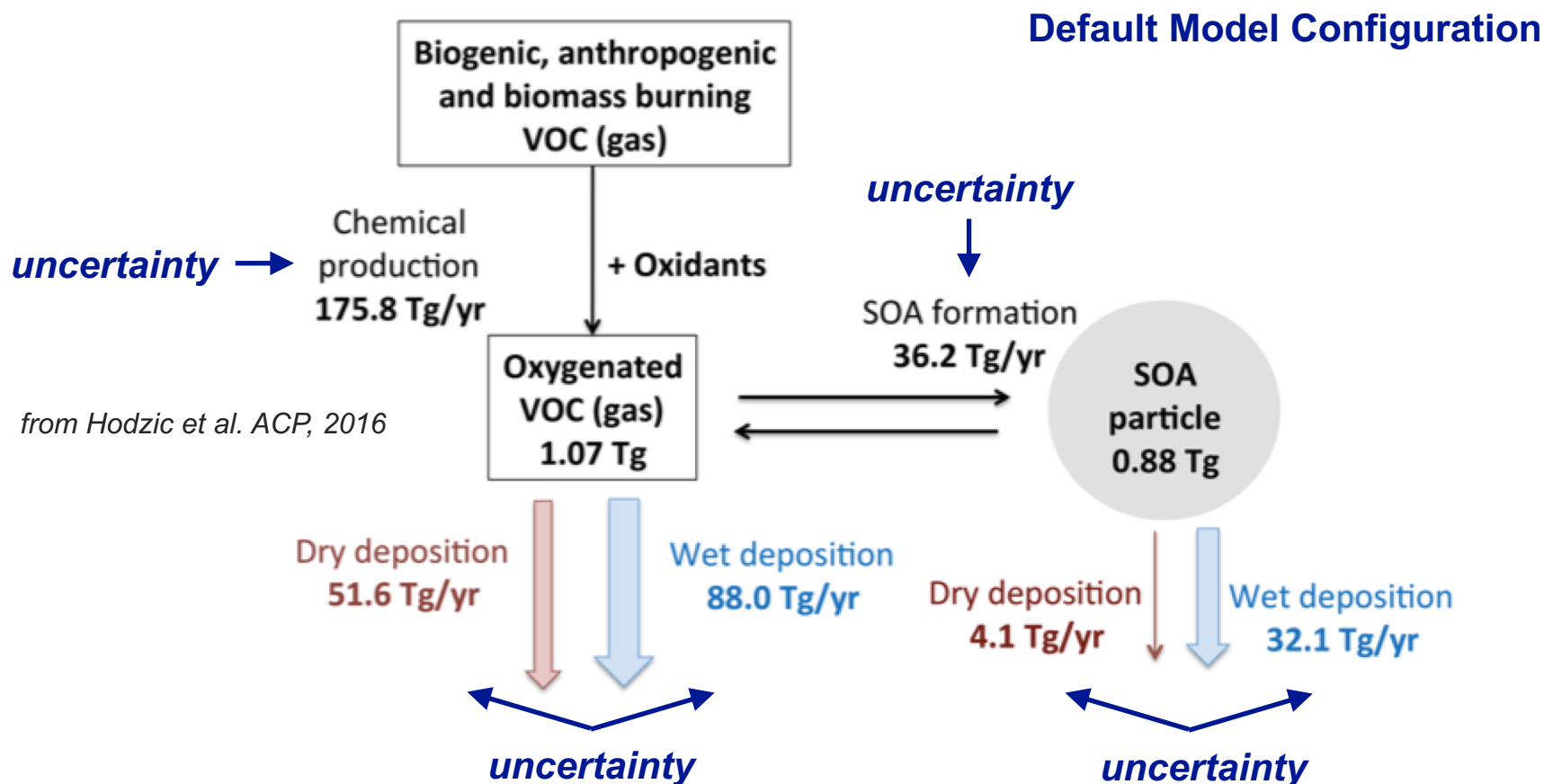


MODIS AOD March 10, 2006



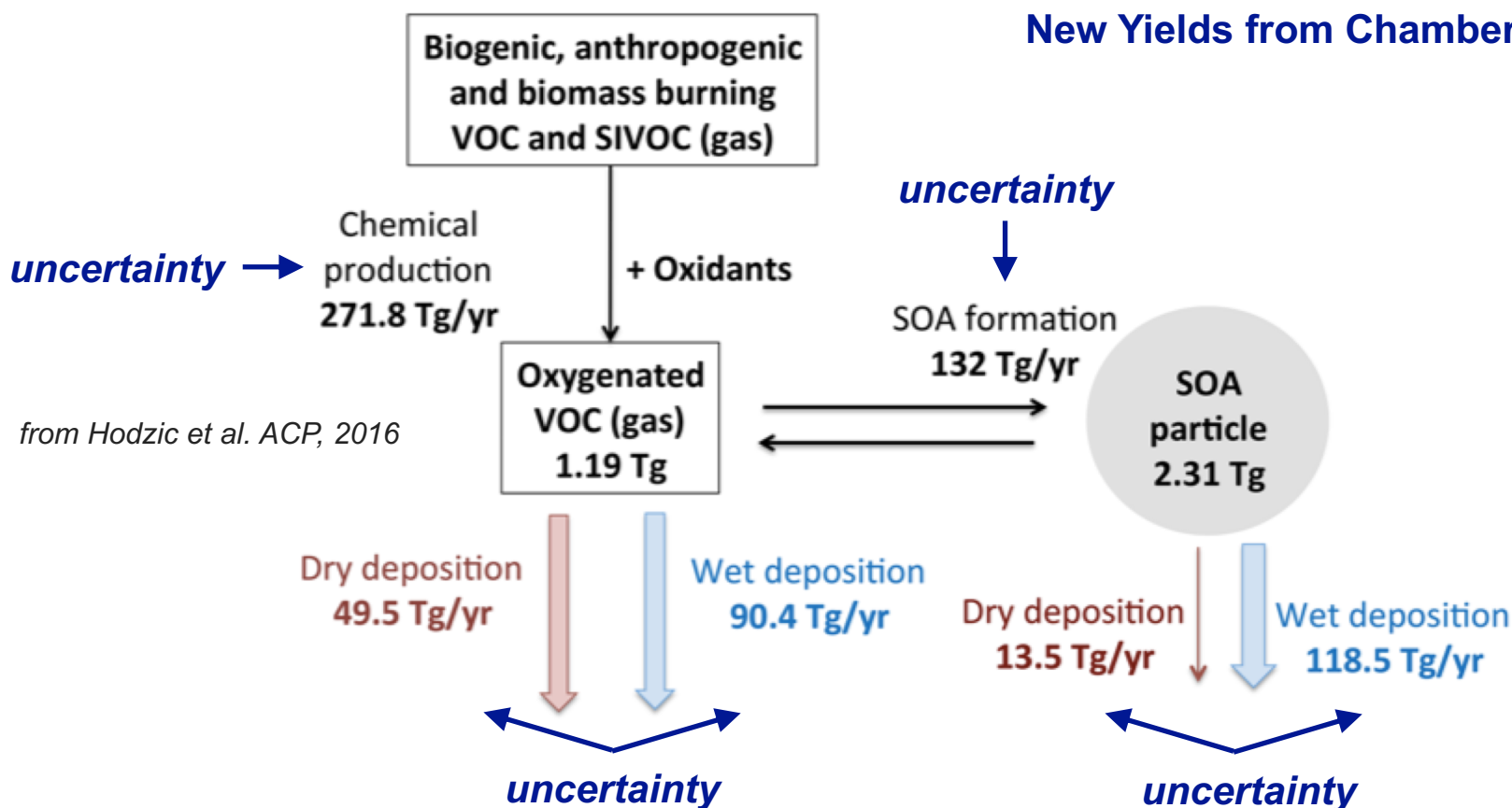
Deposition and the OA Budget

Since organic aerosols (OA) are a large fraction of the fine mode mass, it is important to understand and represent the processes affecting the global budget of OA.



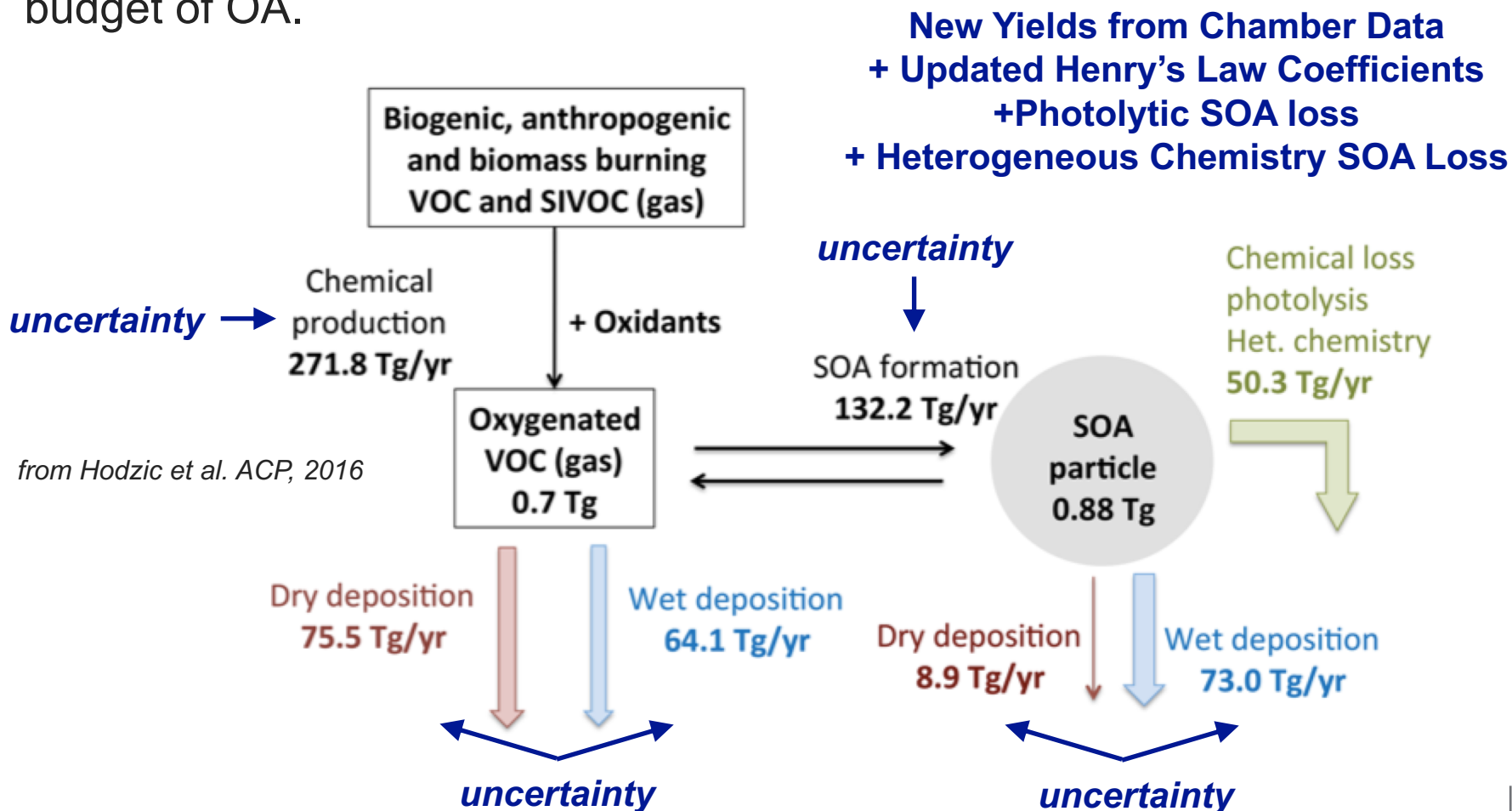
Deposition and the OA Budget

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Deposition and the OA Budget

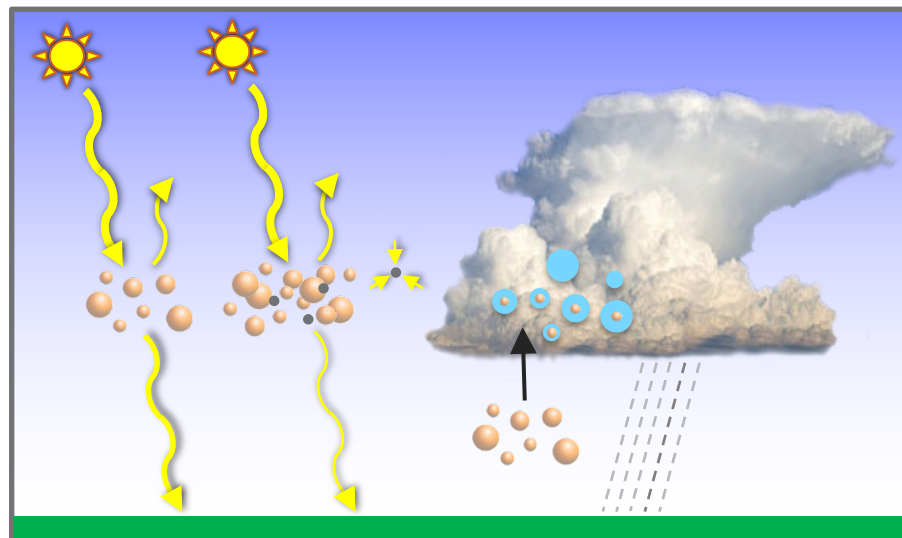
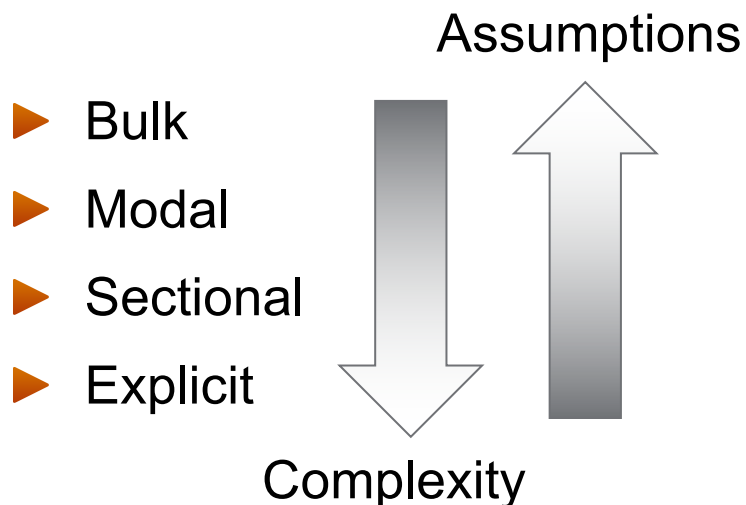
Since organic aerosols (OA) are a large fraction of the fine mode mass, it is important to understand and represent the processes affecting the global budget of OA.



Representation of Aerosol Size, Mixing State, and Morphology

Representing Aerosol Size Distribution

There are 4 basic approaches used to represent the aerosol number and mass size distributions in models



moments:

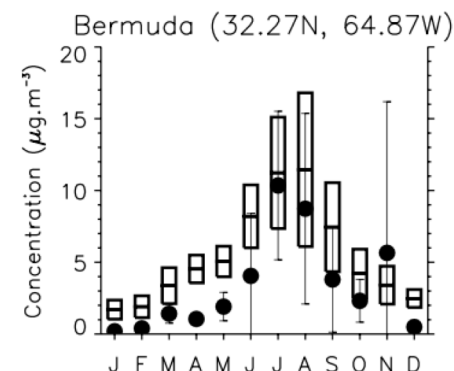
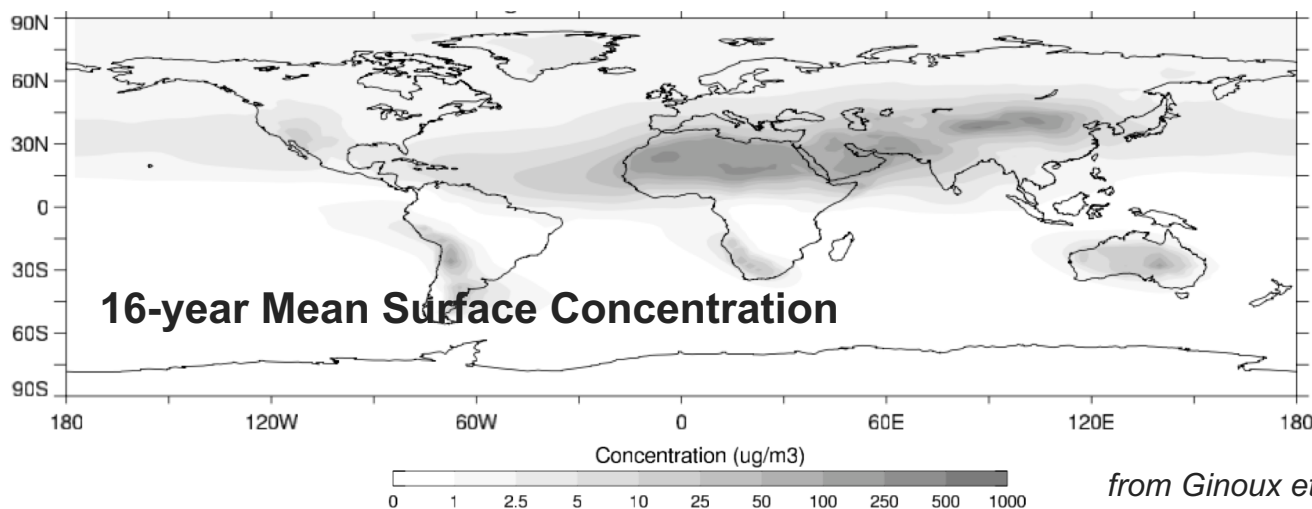
- 1) mass,
- 2) mass & number,
- 3) mass, number, & surface area

Size is important since it affects 1) **radiation** via aerosol optical properties and 2) **clouds** via cloud condensation nuclei (CCN). Also important in terms of **human health**, since smaller particles have a higher probability of penetrating deeper into the lungs.

Size Distribution: Bulk

- ▶ Only total mass of aerosol compounds are represented
- ▶ No information on particle # or size
- ▶ Assume size distribution for radiative transfer and response of cloud properties to aerosol number
- ▶ Numerically efficient

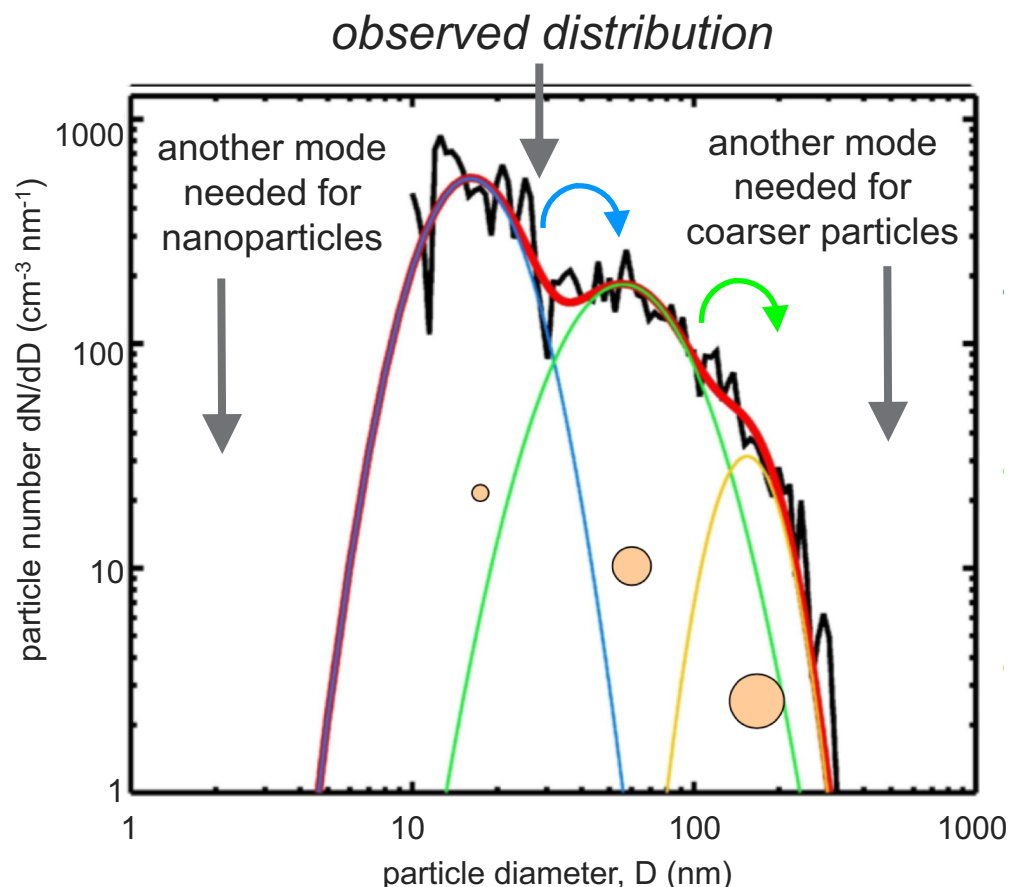
Example: GOCART (Goddard Chemistry Aerosol Radiation & Transport model, Chin et al. JGR 2000)



from Ginoux et al. EMS, 2004

Size Distribution: Modal

- ▶ Represent the size by a discrete number of log-normal distributions
- ▶ Modes smoother than observed distributions
- ▶ Numerical efficient – suitable for AQ and climate models



Example: MAM in CESM

Liu et al. GMD, 2016

4 bins by default

$$\frac{dN}{dD} = \frac{dN}{dD} + \frac{dN}{dD} + \frac{dN}{dD}$$

$$\frac{dN}{dD} \rightarrow N = 8195 \text{ cm}^{-3}$$
$$\mu = 18.22 \text{ nm}$$
$$\sigma = 1.42$$

Aiken
mode

$$\frac{dN}{dD} \rightarrow N = 12732 \text{ cm}^{-3}$$
$$\mu = 68.44 \text{ nm}$$
$$\sigma = 1.57$$

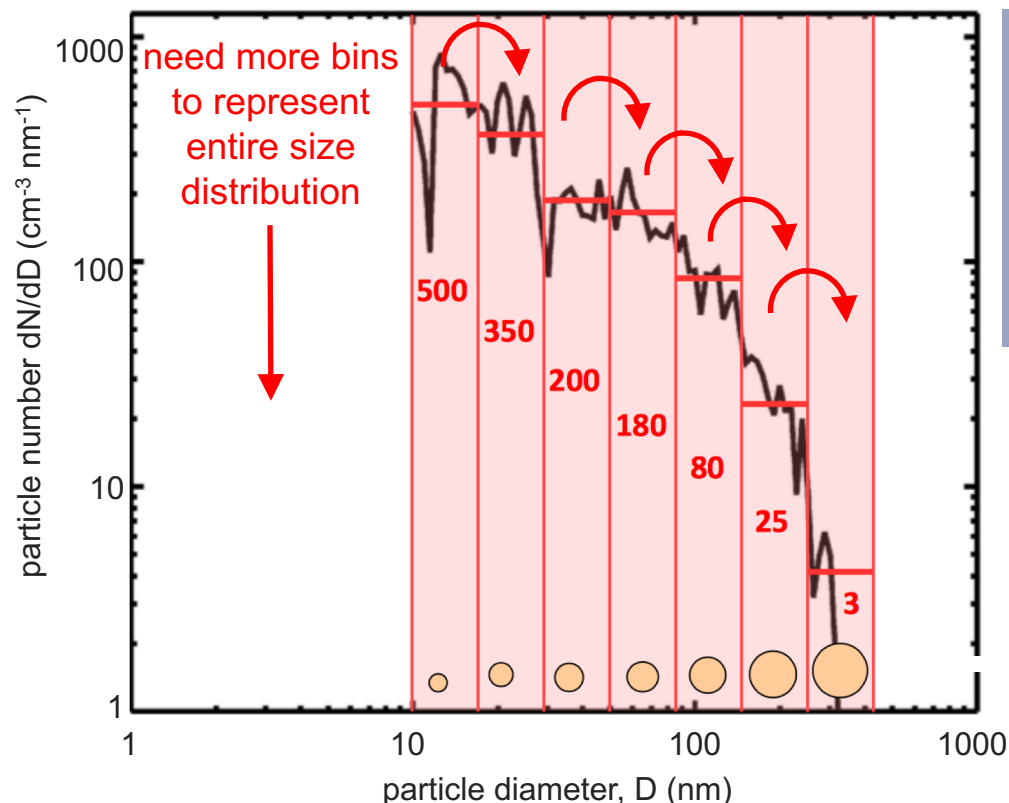
Accumulation
mode

$$\frac{dN}{dD} \rightarrow N = 3140 \text{ cm}^{-3}$$
$$\mu = 164.41 \text{ nm}$$
$$\sigma = 1.28$$

Coarse
mode

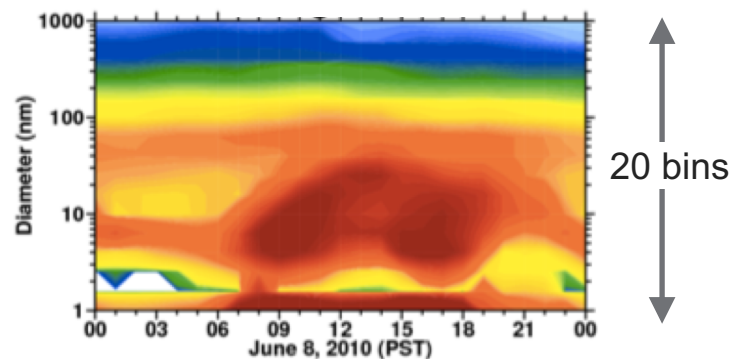
Size Distribution: Sectional

- ▶ Represents the size distribution by a discrete number of size bins
- ▶ More flexible than modal approach – better represents size
- ▶ Need a large number of bins to represent observed distributions
- ▶ Numerical more expensive - suitable for AQ models and research studies



Example: MOSAIC in WRF-Chem
Zaveri et al. JGR, 2008

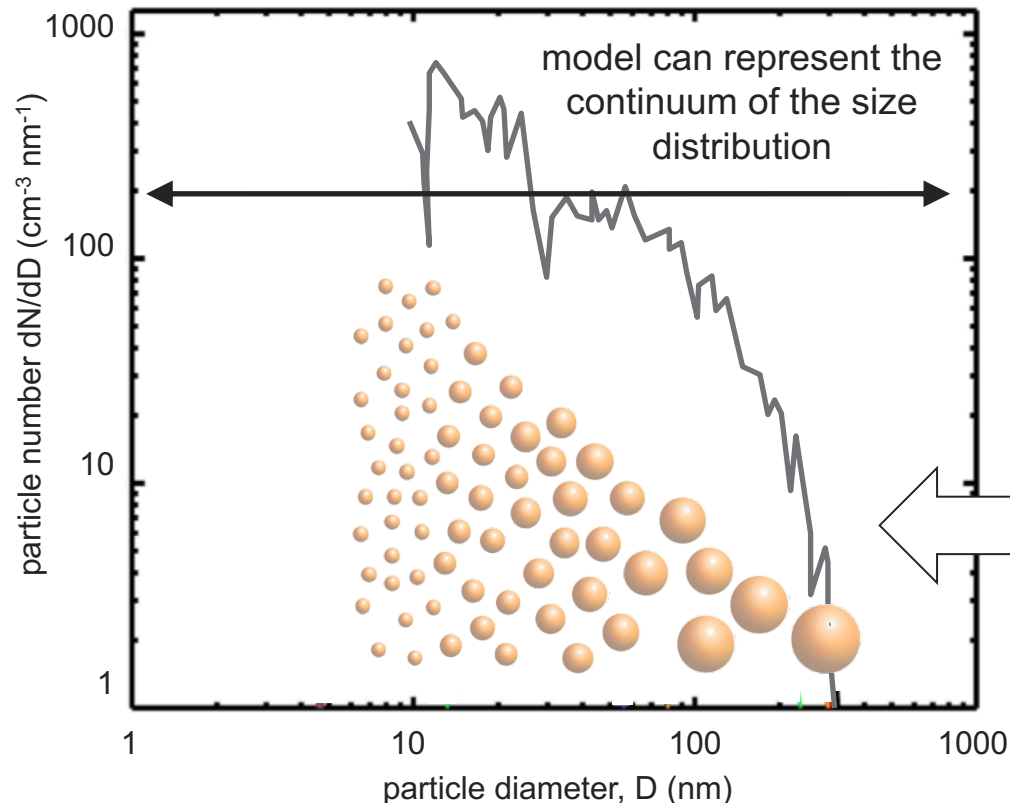
4 or 8 bins by default but can be configured to any #



from Lupascu et al. ACP, 2015

Size Distribution: Explicit

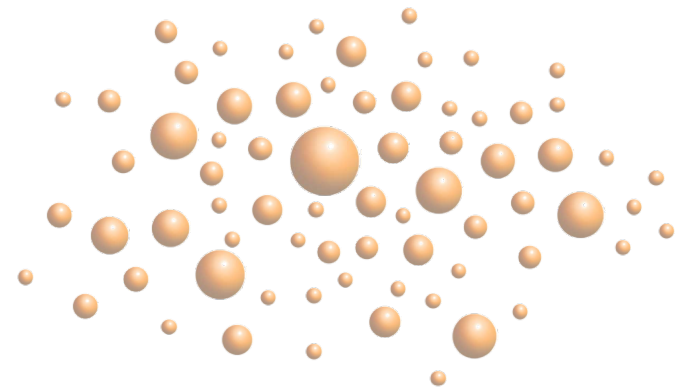
- ▶ Represents the size distribution by explicitly simulating each particle in a population of particles. Need to simulate thousands of particles.
- ▶ More flexible than both modal and sectional approaches
- ▶ Numerical most expensive - suitable for research studies



Example: PartMC-MOSAIC

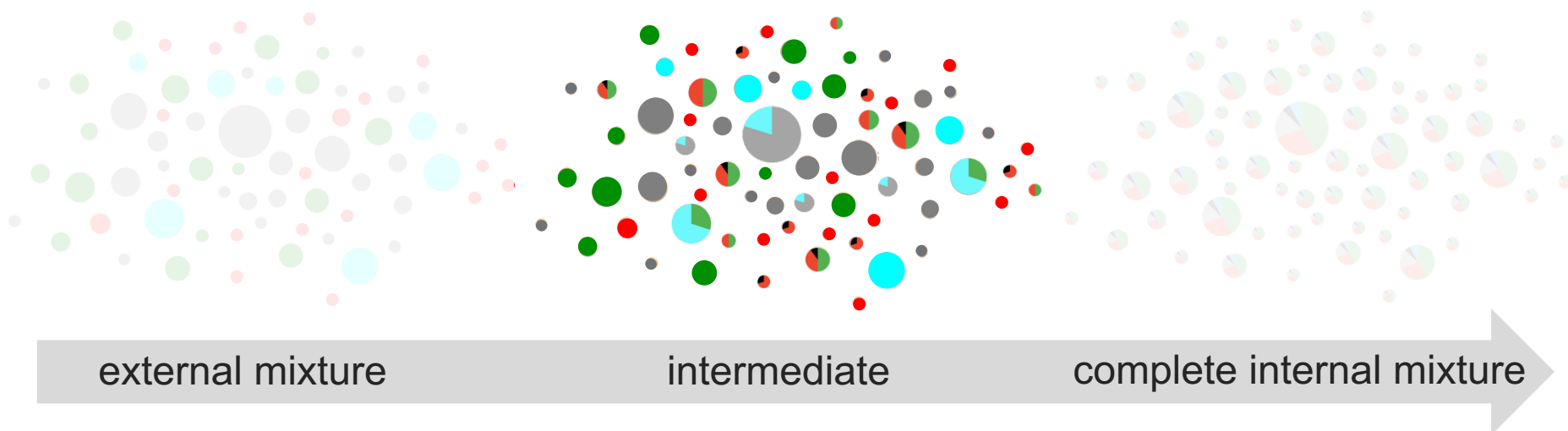
Riemer et al. JGR, 2010

Zaveri et al. JGR, 2010



Mixing State: Definition and Importance

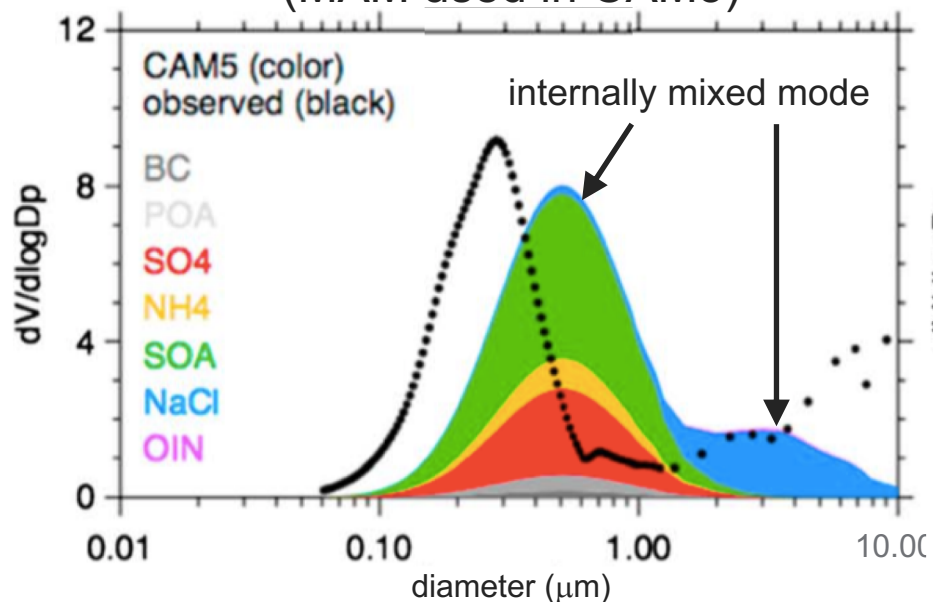
An Overly Simplistic Depiction, Where Color = Composition



- ▶ In the real world, particles are mostly externally mixed after emission or nucleation. Then, they undergo coagulation and chemical aging so that population becomes more internal mixed over time.
- ▶ Except for explicit aerosol models, assumptions are made to treat the aerosol mixing state
- ▶ Assumptions in the aerosol mixing state can significantly affect estimates of absorption and and CCN concentrations (e.g. Ching et al. ACP, 2017)

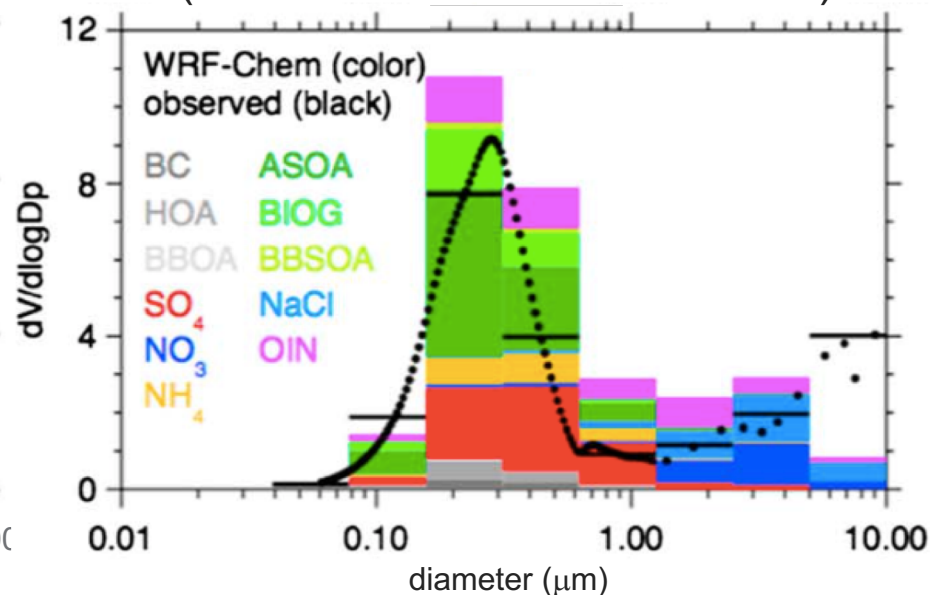
Model Representations of Mixing State

Modal Approach
(MAM used in CAM5)



- ▶ Constant composition fraction in each mode, but can vary by mode.
- ▶ Each mode is internally mixed
- ▶ Hydrophobic mode of BC that can transition into hydrophilic mode of BC over time to account for aging

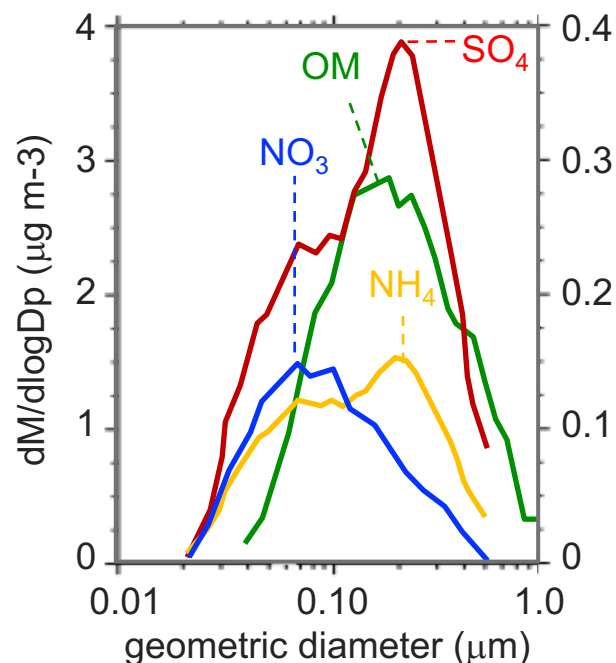
Sectional Approach
(MOSIAC used in WRF-Chem)



- ▶ Constant composition fraction in each bin, but can vary by bin.
- ▶ More detailed representation permits fractional composition to vary by size over smaller changes in particle diameter

Observations of Mixing State

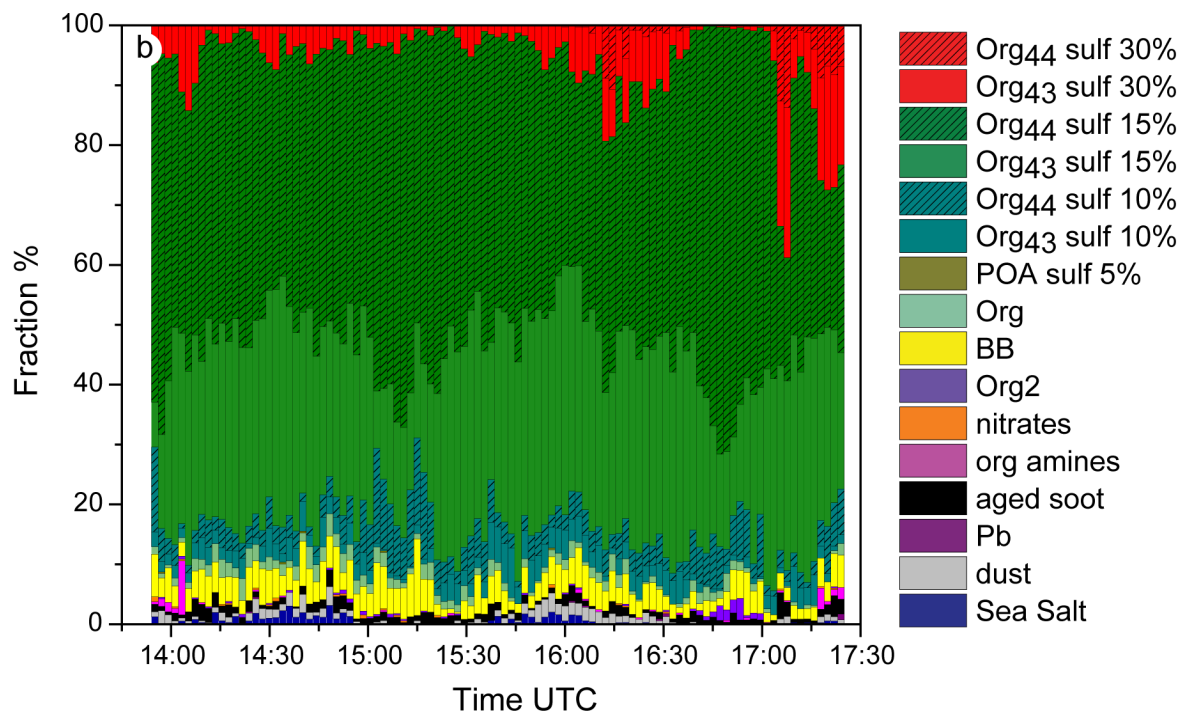
AMS Measurements
(bulk mass spectrometer)



from Fast et al. ACP, 2014

Shows that composition size distribution is not the same for various species

SPLAT Measurements
(single particle mass spectrometer)



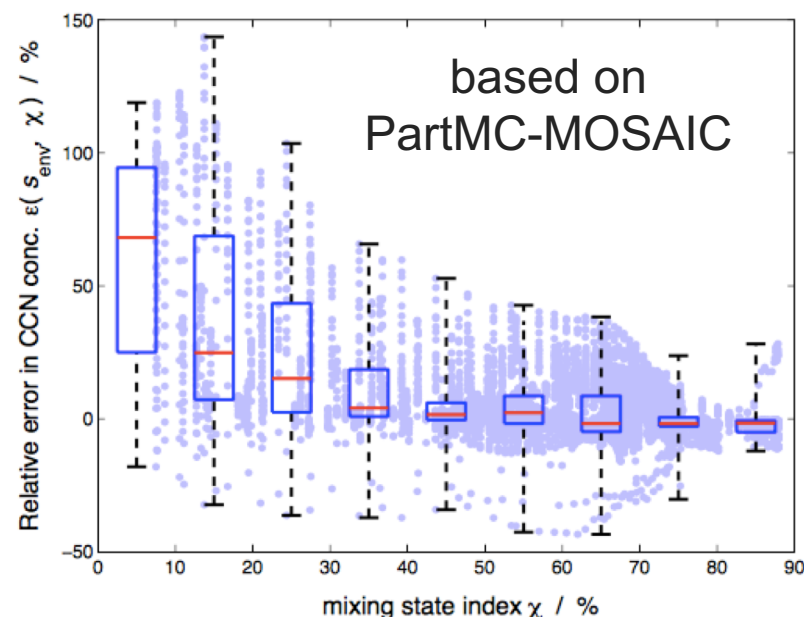
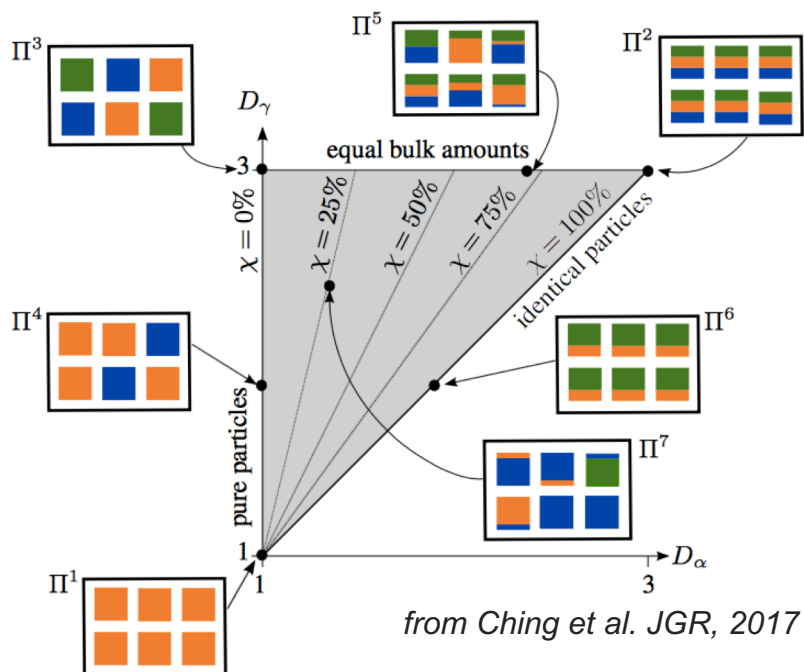
from Berg et al. JGR, 2016

Shows that composition is very complex. Except for explicit treatments, current models cannot represent this level of complexity.

Quantification of Mixing State

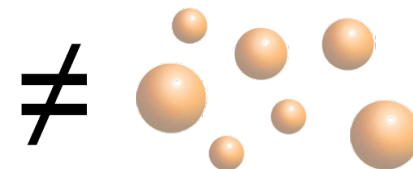
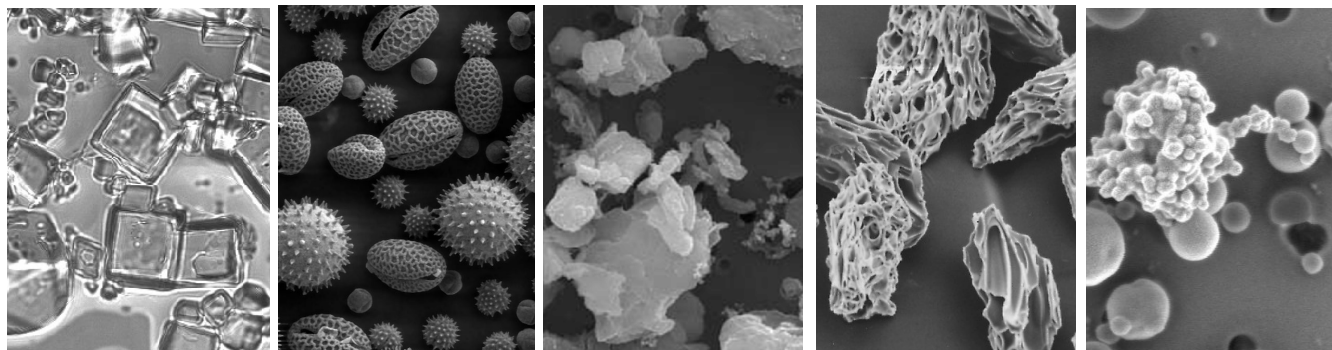
► New metrics being developed to quantify the degree of internal mixing

► Riemer and West, ACP (2013) proposed: $\chi = \frac{D_\alpha - 1}{D_\gamma - 1}$, = 0 for external
= 1 for internal



mixing state information becomes
unimportant for more internally-
mixed populations

Aerosol Shape: The Next Frontier

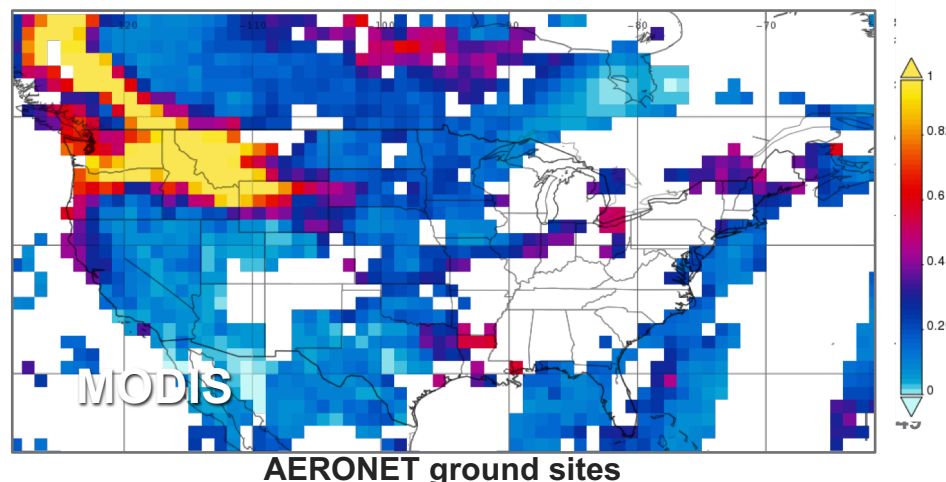
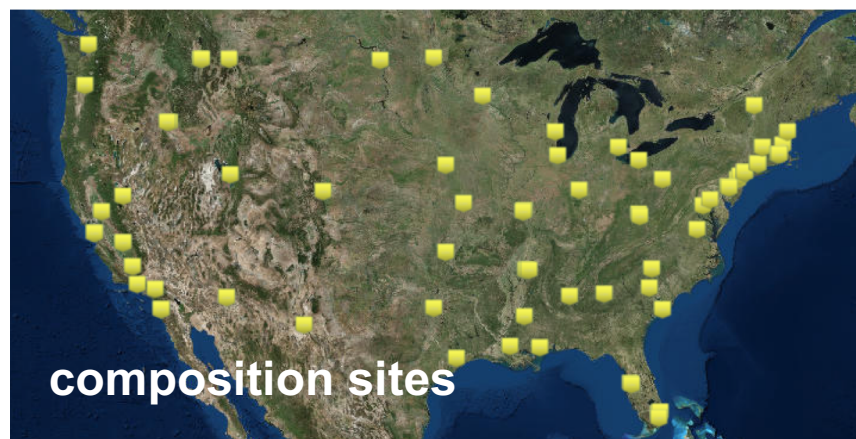
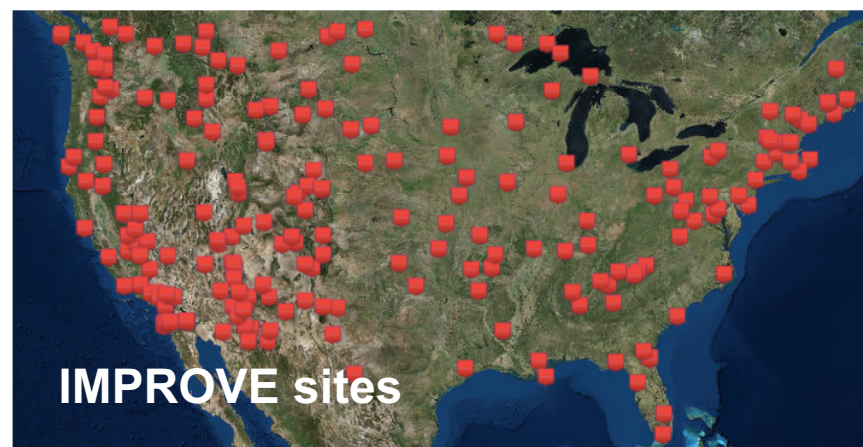


- ▶ Models assume particulates are spheres. Of course, many times they are not.
- ▶ Shape can also change in time. Particles become coated by secondary processes that make them more sphere-like. Soot particles are initially complex fractal-like structures that collapse over time.
- ▶ Shape not accounted for by models, even explicit treatments
- ▶ When does shape matter?
 - May affect gas-to-particle partitioning – not strictly a shell-core
 - Affects optical properties, but these effects may cancel each other
 - Irregularities provide contact surfaces where IN preferentially forms

Model Evaluation and Computational Expense

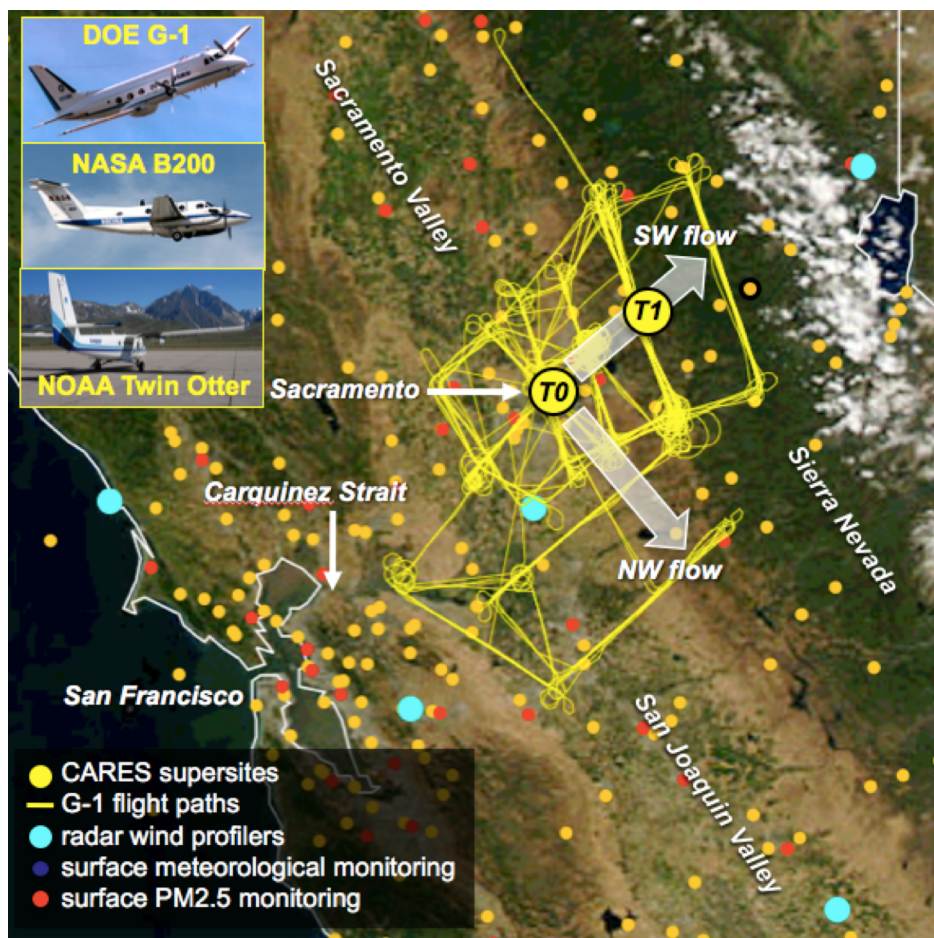
Routine Observations

Routine measurements are available from EPA and NASA to quantify model performance, but they are limited to **bulk quantities** at the surface or column integrated quantities (e.g. AOD and other optical properties)



Field Campaign Observations

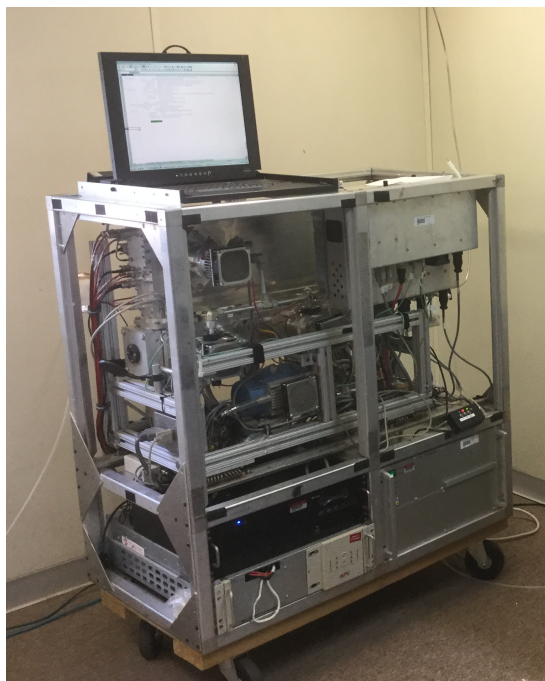
Field campaign research measurements, available from several agencies, can be used to quantify model performance. They have **more detailed information on aerosol properties** than available from routine monitoring.



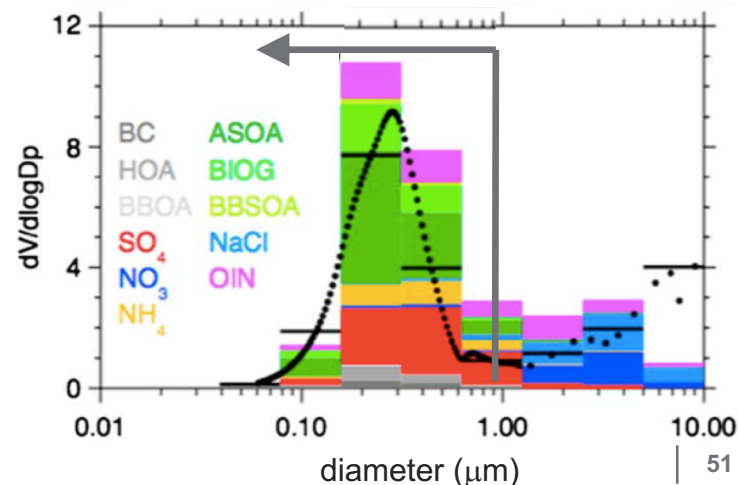
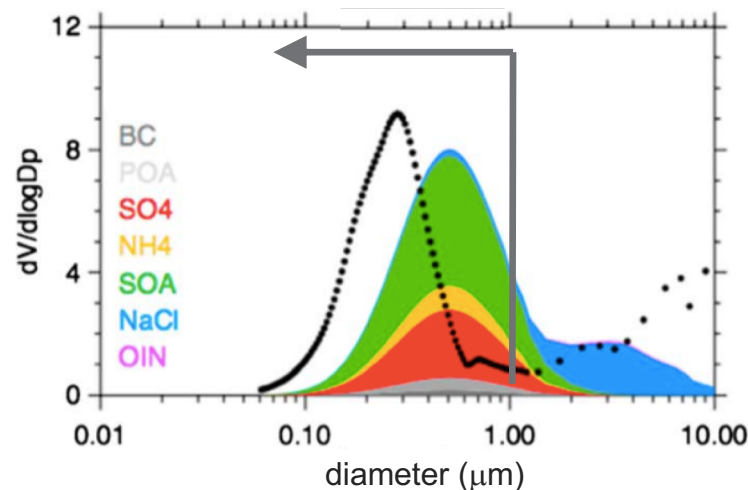
- ▶ Number (multiple types)
- ▶ Size distribution (multiple types)
- ▶ Composition (AMS, single particle, SP2)
- ▶ Morphology and composition (SEM)
- ▶ Optical properties (multiple types)
- ▶ Trace gases: standard suite, PTR-MS, CIMS, etc. for aerosol precursors

Measured and Modeling Quantities are Not Necessarily the Same Thing

Sometimes, evaluating aerosol models with data is like **comparing apples with oranges**. One example is associated with AMS measurements:



need to obtain a similar size range from the model to compare with the measurements



- ▶ Measures PM1 ($0.04 < D_p < 1 \mu\text{m}$), but ...
- ▶ Depends on "collection efficiency"
- ▶ Needs to check consistency with other size data

Measurement Uncertainties

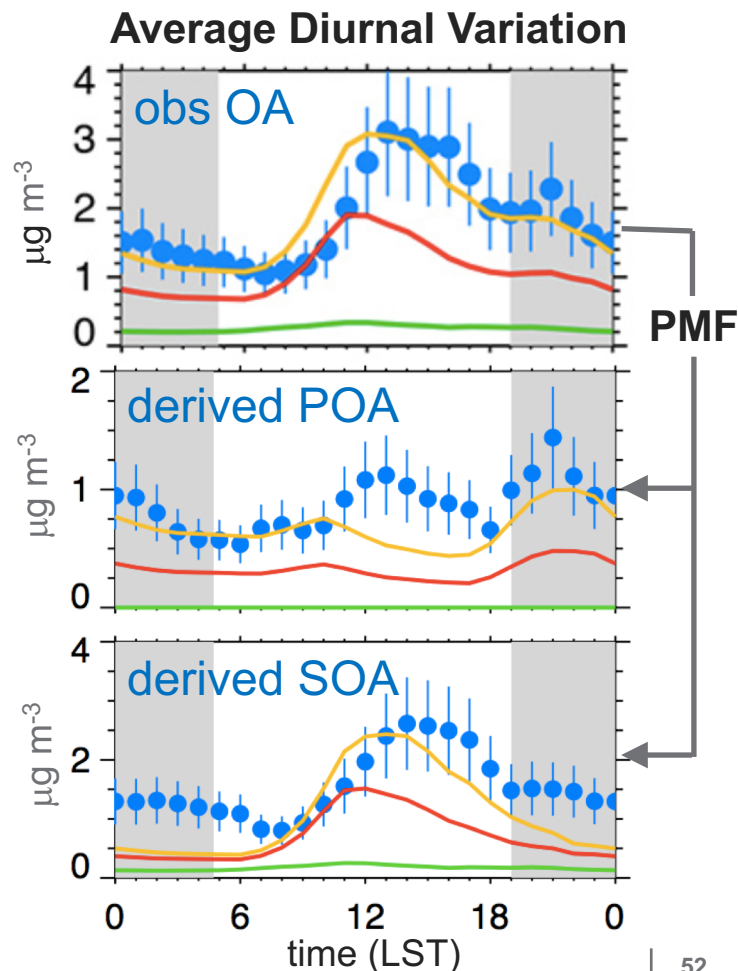
Another important consideration often ignored by modelers is **measurement uncertainty**, especially for state-of-the-science instrumentation.



need to include data uncertainty wherever possible, but that can often be problematic

←→
uncertainty propagates to derived quantities

- ▶ Detection limit of 2.9 nm m^{-3} , but ...
- ▶ Uncertainty difficult to quantify because it depends on aerosol properties (Takegawa et al. AST, 2005). User estimates vary widely.



from Fast et al. ACP, 2014

User Considerations for Modeling Aerosols

- ▶ What is the **problem** being addressed by the aerosol model?
- ▶ What level of **complexity in size distribution** is needed?
- ▶ How many **aerosol (and trace gases) species** are needed?
- ▶ What is the **domain extent**, **spatial resolution**, and the **time period** needed to represent the processes of interest?
- ▶ Do I need to include aerosol-radiation-cloud-precipitation **feedbacks**?
- ▶ How much **disk space** can I afford?
- ▶ How long am I willing to wait for one simulation to finish? Am I a patient person?



Inevitably, there is always a trade off between spatial resolution, simulation length, level of model complexity, and your sanity.

It's All About the Cost of Advection: Mechanisms in WRF-Chem

simple

handling cloud-borne aerosol

▶ **MOZART (82) + GOCART (15) = 97 species**

BC(2), OC(2), dust(5), sea-salt(4), other(2)

▶ **RADM2 (42) + MADE/SORGAM (38) = 80 species + 38**

BC(2), SO₄(2), NH₄(2), NO₃(2), Na(2), Cl(2), sea-salt(1), OM(18), dust(2) other(2), number(3)

▶ **RACM (65) + VBS SOA (38) = 134 species + 40**

BC(2), SO₄(2), NH₄(2), NO₃(2), Na(2), Cl(2), sea-salt(1), OM(18), dust(2) other(2), number(3)

▶ **MOZART (136) + MOSAIC 4 size bins (64) = 200 species + 56**

BC(4), SO₄(4), NH₄(4), NO₃(4), Na(4), Cl(4), OM(20), Ca(4), dust(4), water(8), number (4)

▶ **SAPRC (97) + MOSAIC 4 size bins (112) = 209 species + 108**

BC(4), SO₄(4), NH₄(4), NO₃(4), Na(4), Cl(4), OM(68), Ca(4), dust(4), water(8), number (4)

▶ **SAPRC (97) + MOSAIC 8 size bins (216) = 313 species + 200**

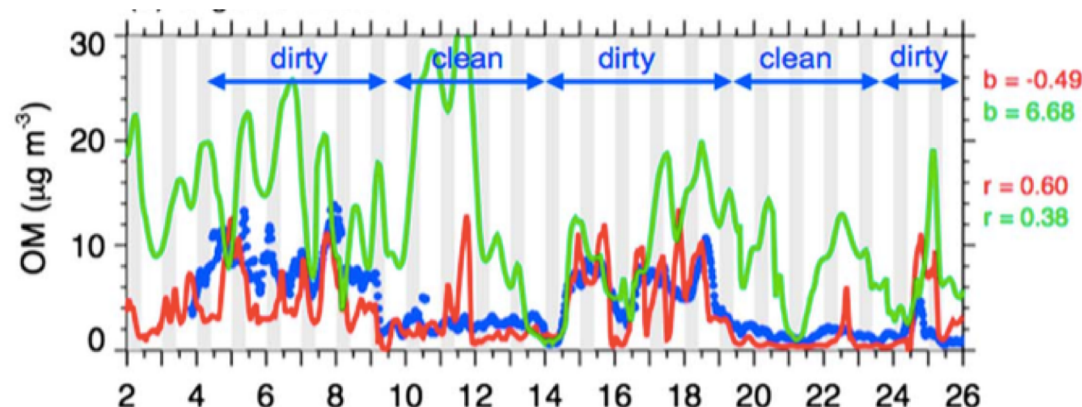
BC(8), SO₄(8), NH₄(8), NO₃(8), Na(8), Cl(8), OM(136), dust(8), water(16), number(8)

complex

Finally, My Perspective on Model Evaluation

- ▶ Given the complexity of aerosol processes and our ability to represent those processes in models, it is amazing how well predicted aerosol properties are **(sometimes)**

observed
WRF-Chem
CAM5



- ▶ Of course, a good simulation does not mean that the model is a true representation of reality. It is possible to **“get the right answer for the wrong reasons”**.
 - *Should view a good model simulation with skepticism*
 - *Check all components of the modeling system, e.g. meteorology*
- ▶ On the other hand, aerosol predictions often have large errors so that one should expect that **errors in aerosol predictions are relatively higher** than those associated with meteorology and trace gases

Pandora's Box / Aerosol Modeling

uncertainties in emissions

strange model behavior

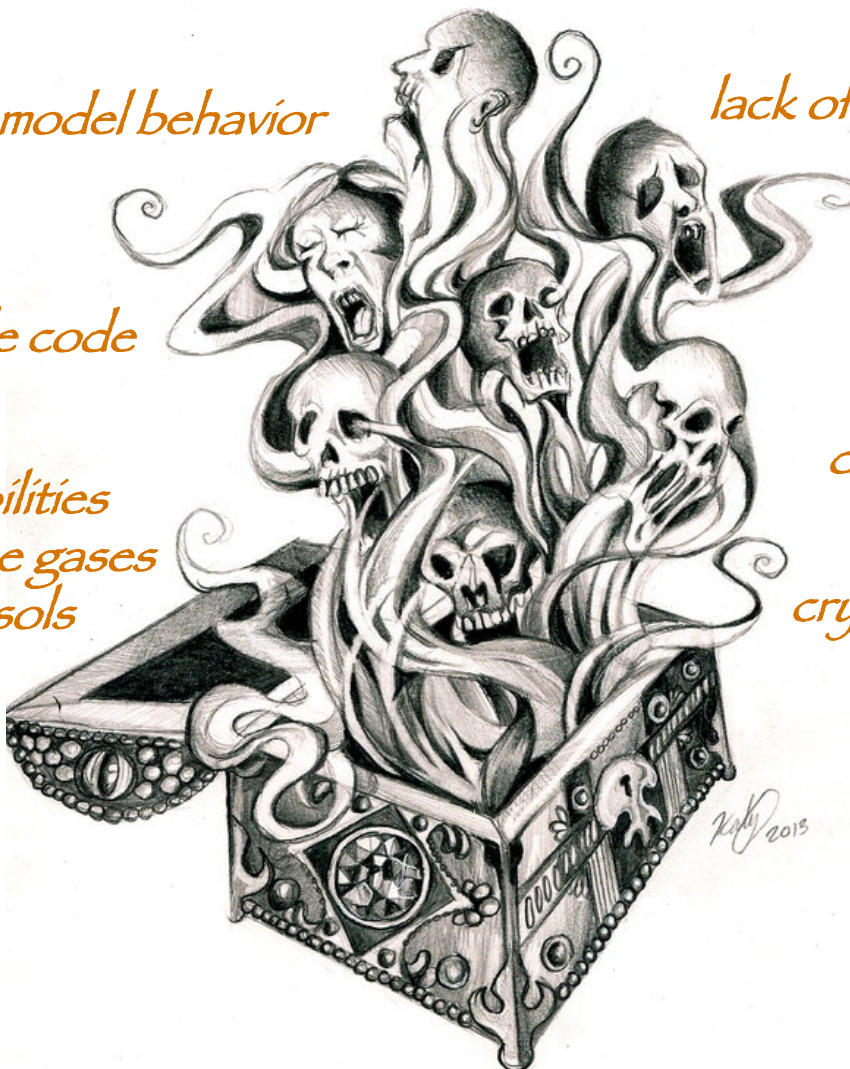
lack of documentation

indecipherable code

*differences between
journal article
description and actual
code*

*incompatibilities
between trace gases
and aerosols*

*cryptic names for
parameters*



Research Opportunities at PNNL

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- ▶ www.pnnl.gov/atmospheric/jobs.asp

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- Atmospheric Data Analyst
- Earth Scientist, Cloud-Aerosol Interactions
- Postdocs
- etc.

- ▶ Contact our recruiter:
Gary Worrell
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