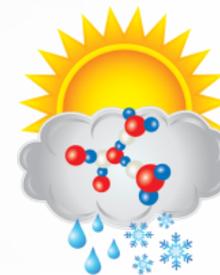


Using the Aerosol Modeling Testbed for ASR Focus Groups

Jerome Fast

- ▶ Overview of AMT
- ▶ Applications
 - *New Particle Formation – official focus group*
 - *Aerosol Mixing State – official focus group*
 - *Secondary Organic Aerosol – potential focus group*
- ▶ Challenges



ASR
Atmospheric
System Research

What is a Testbed?

- ▶ **According to Wikipedia, a testbed is** *“a platform for experimentation of large development projects. Testbeds allow for rigorous, transparent, and replicable testing of scientific theories, computational tools, and new technologies.”*

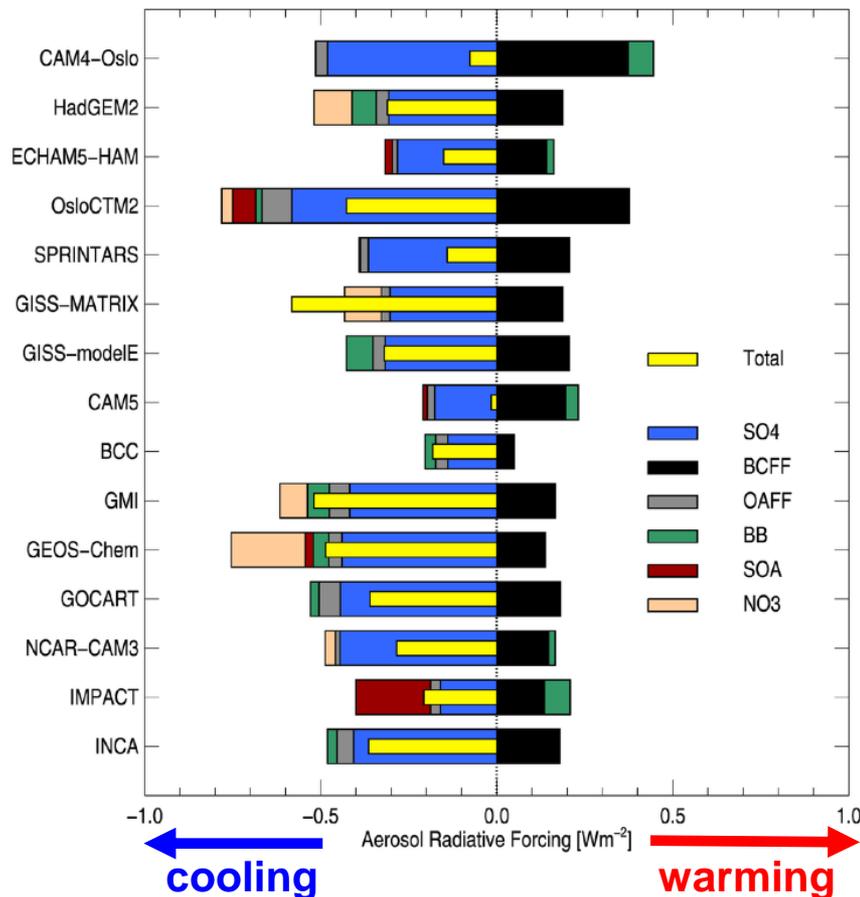
*“The term is used across many disciplines to describe a development environment that is shielded from the hazards of testing in a live or production environment. It is a method of **testing a particular module** (function, class, or library) in an isolated fashion ... A testbed is used as a proof of concept or when a **new module is tested apart from the program/system it will later be added to ...**”*

- ▶ **AEROCOM** (AEROSol COMparisons between observations and models) is an example that focuses on global model performance and uses mostly satellite data and a limited number of surface networks

Why are Testbeds Useful for the Aerosol Modeling Community?

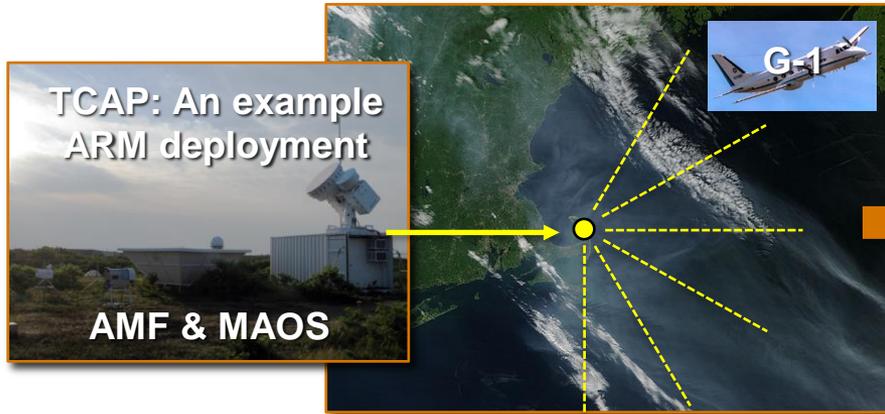
Global and Annual Mean Radiative Forcing in AEROCOM Phase II

from Myhre et al., ACP, 2013



- ▶ **Aerosol burden differs** by a factor of 2 – 3 among the models and estimates of **direct radiative forcing** varies (0 to -0.5 W m^{-2})
- ▶ Differences among the models are **due to many sources** (emissions, meteorology, configuration) rather than just the treatment of aerosols
- ▶ While these model comparisons are useful, they contain **little insight on how to better represent aerosol properties**
- ▶ Evaluating global models with ARM field campaign data (that often have the most detailed aerosol property measurements) **is problematic**

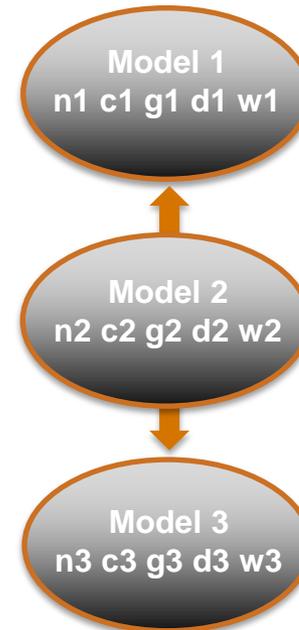
Moving Towards A New Modeling Paradigm



The **AMT** is a framework that streamlines the process of testing and evaluating **aerosol and cloud process modules** over a range of spatial / temporal scales

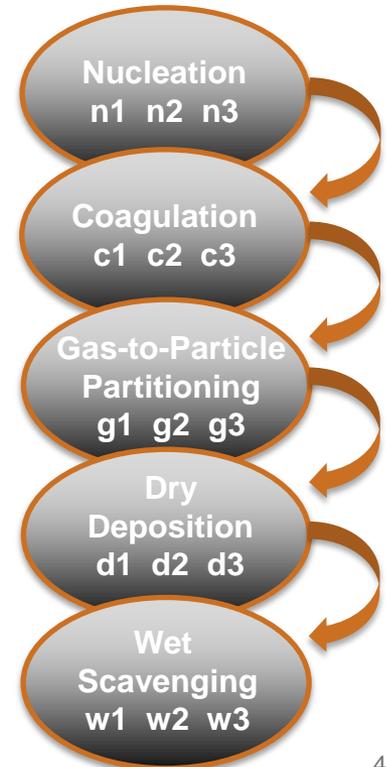
- ▶ **Systematically and objectively** evaluate aerosol process modules using both extensive field campaign and operational data
- ▶ **Provide tools** that facilitate science by minimizing redundant tasks
- ▶ **Document performance** in relation to computational expense
- ▶ **Foster collaboration** – like AEROCOM but at regional scales

Traditional Modeling Paradigm



e.g. model inter-comparison studies

New Modeling Paradigm



Host Model:

- ▶ Version of WRF-Chem – more interoperable to simplify implementation of new modules and targets aerosol processes

Testbed Cases:

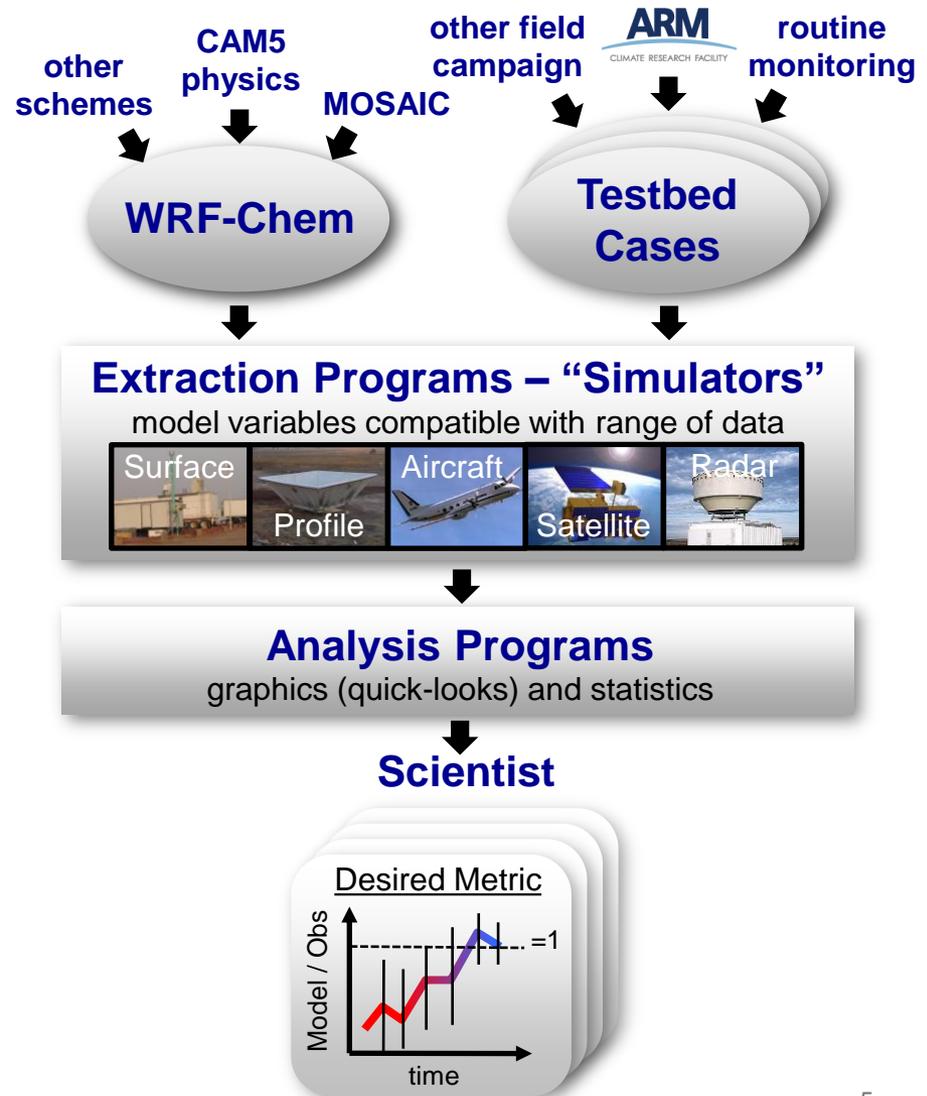
- ▶ Sets of field campaign data coupled with long-term monitoring data targeting specific processes that affect the aerosol lifecycle

Community Tools:

- ▶ Suite of tools that graphically and statistically compare a wide range of observed and simulated quantities=

Long-Term Archive (aspiration):

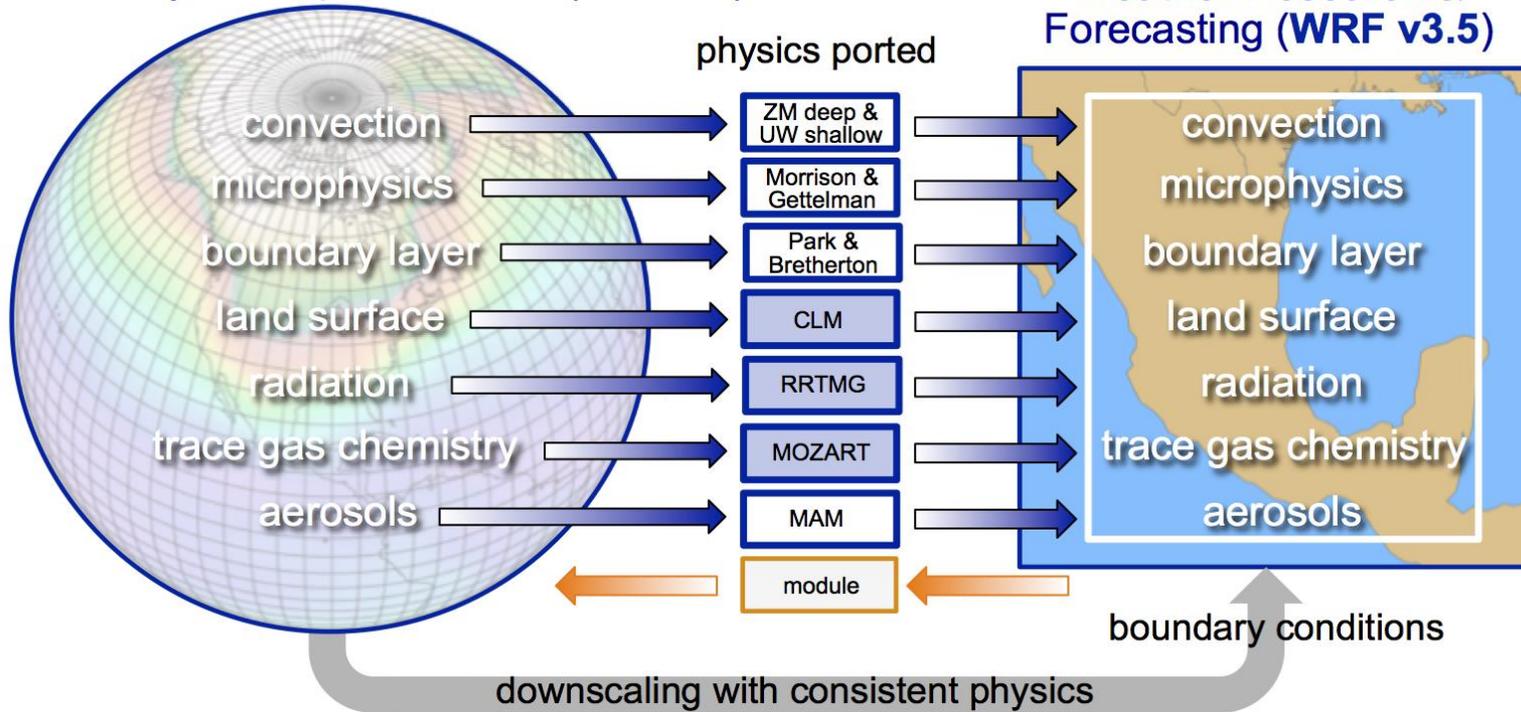
- ▶ Goal of documenting performance over time and useful for data mining by non-modelers



Evaluation of CAM5 Physics at Higher Spatial Resolution

Community Atmosphere Model (**CAM5.1**)

Weather Research & Forecasting (**WRF v3.5**)



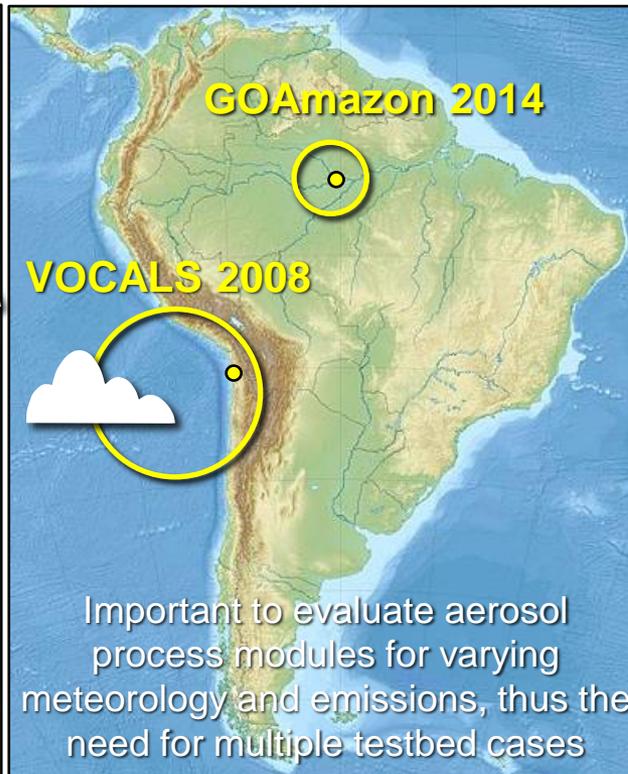
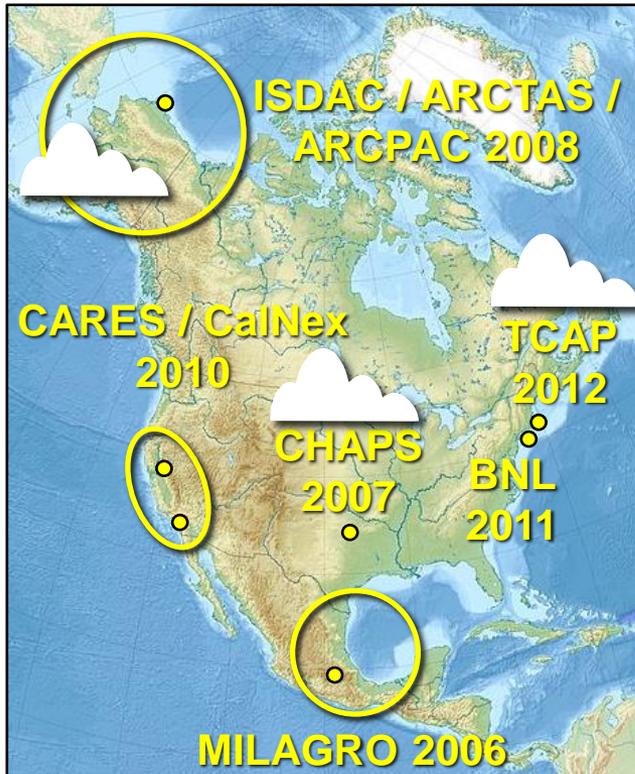
- ▶ Aerosol Models in WRF: **GOCART**, **MAM**, **MADE/SORGAM**, **MOSAIC**



- ▶ Others ported (not in public version): **APM** (GEOS-Chem), **MADRID** (CMAQ), **MOSAIC-PDFITE** (Univ. Manchester), **MOSAIC-UT** (Univ. Tokyo)



Testbed Cases: Datasets



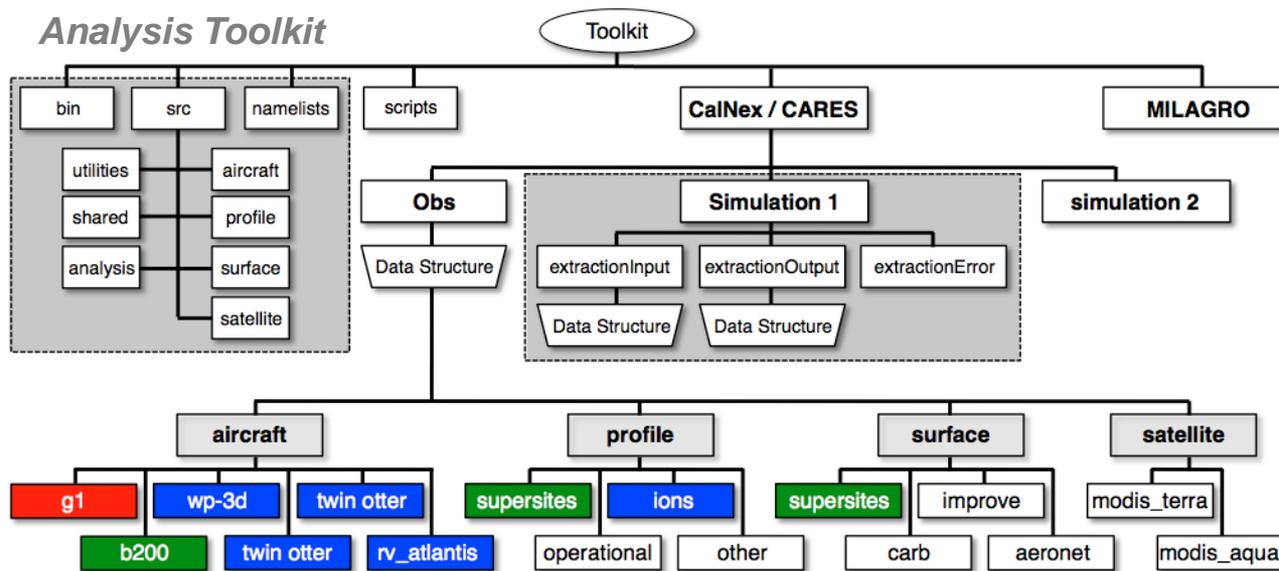
Characterization of aerosol microphysics, optical, and cloud nucleating properties at the surface and aloft using advanced instrumentation, e.g.

- Aerosol Mass Spectrometer (AMS)
- Single particle soot photometer (SP2)
- Single particle instruments (SPLAT, ATOFAMS, PALMS)
- Photoacoustic soot photometer
- Cavity ring-down spectroscopy
- High Spectral Resolution Lidar

However the AMT utilizes a wide range of meteorological (including clouds) and trace gas measurements as well.

- ▶ Nearly complete cases; **MILAGRO, CARES/CalNex, BNL**
- ▶ Several planned cases: **TCAP, GOAmazon...**
- ▶ Partially complete cases: **CHAPS, ISDAC, VOCALS**
- ▶ Users developing other cases: **POLARCAT, ...**

- ▶ Each field campaign has data in a varieties of formats and their own idiosyncrasies, which is a time sink for modelers
- ▶ The AMT uses a common directory structure to organize categories of measurements from each field campaign
- ▶ Analysis Toolkit software extracts model variables compatible with data and organizes the model output in the same way

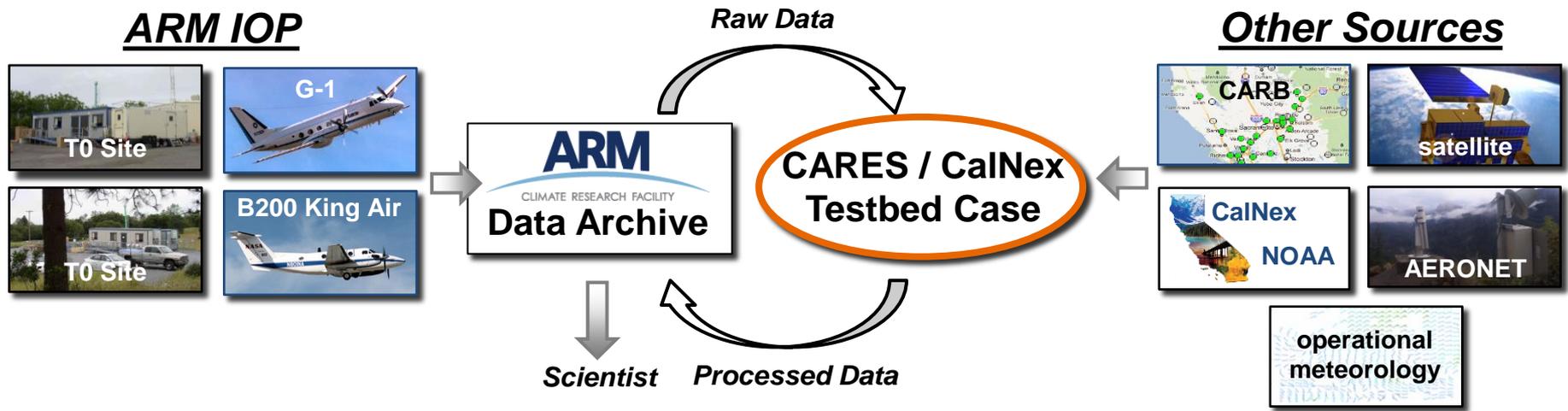


**CARES / CalNex
Example**

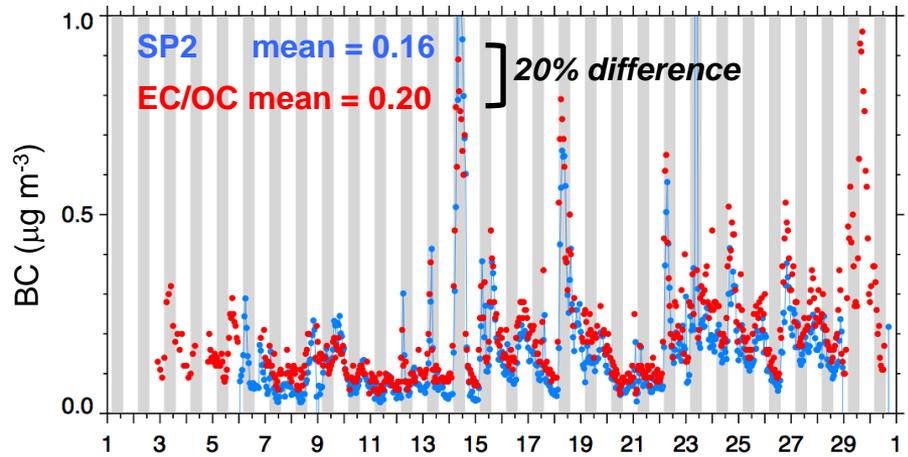
CARES
CalNex
both

- ▶ 'Analysis Toolkit' and Testbed Cases: <http://www.arm.gov/data/eval/59>

Testbed Cases: Data Processing



- ▶ Not simply just collecting data and reformatting ...
- ▶ Additional temporal averaging (dealing with 1-s data), removing bad data, questioning mentors about data details
- ▶ Facilitates data inter-comparisons that are not usually made to better quantify data uncertainties





Using the AMT in its Present Form for ASR Focus Groups

New Particle Formation: Potential ARM Datasets for a Testbed Case

New Particle Formation Study (NPFS)

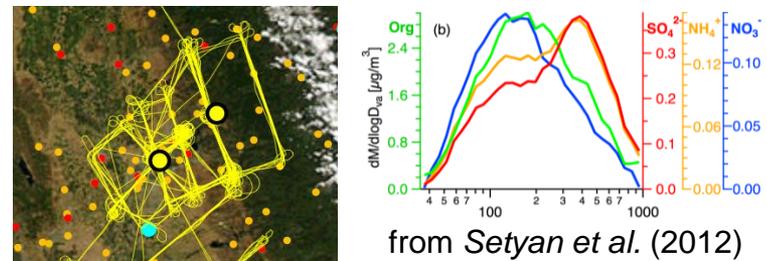
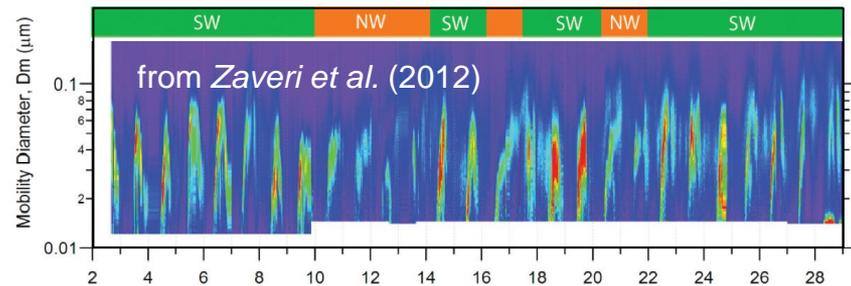
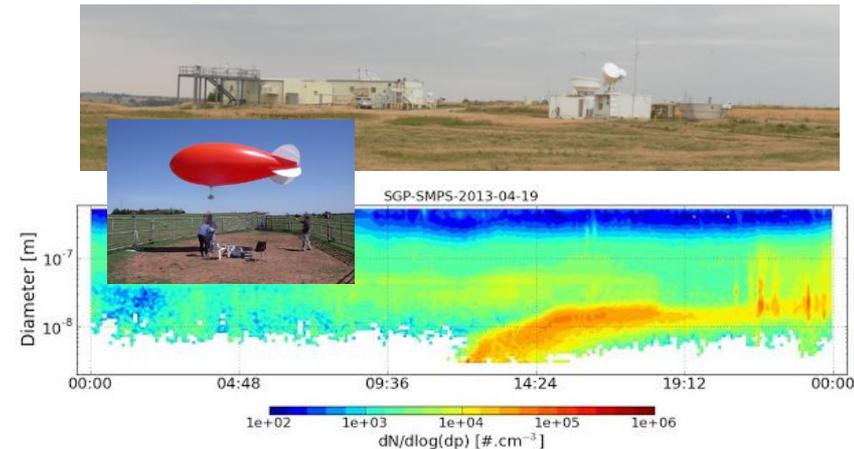
- ▶ SGP central facility, April – May 2013
- ▶ Instruments include nano-aerosol mass spectrometer (NAMS), chemical ionization mass spectrometer (CIMS), ammonia phosphorus mass spectrometer

CARES ?

- ▶ Vicinity of Sacramento, June 2010
- ▶ Many NPF events were observed, but NPF was not an objective and the campaign lacked more detailed measurements like NPFS 2013

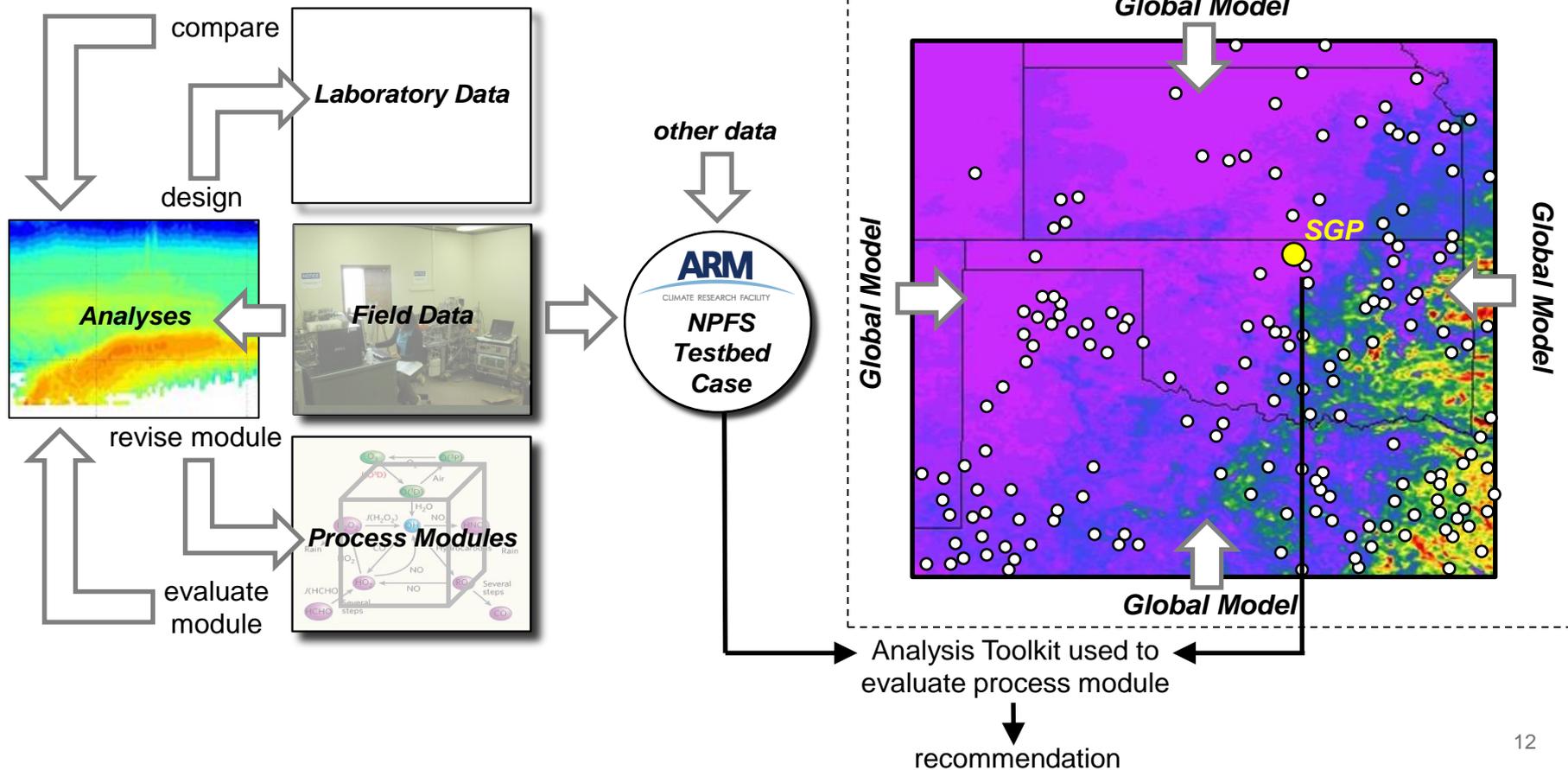
Other Candidates ?

- ▶ Depends on what the focus group wants and can be accomplished in a reasonable time frame (e.g. GOAmazon, MILAGRO)



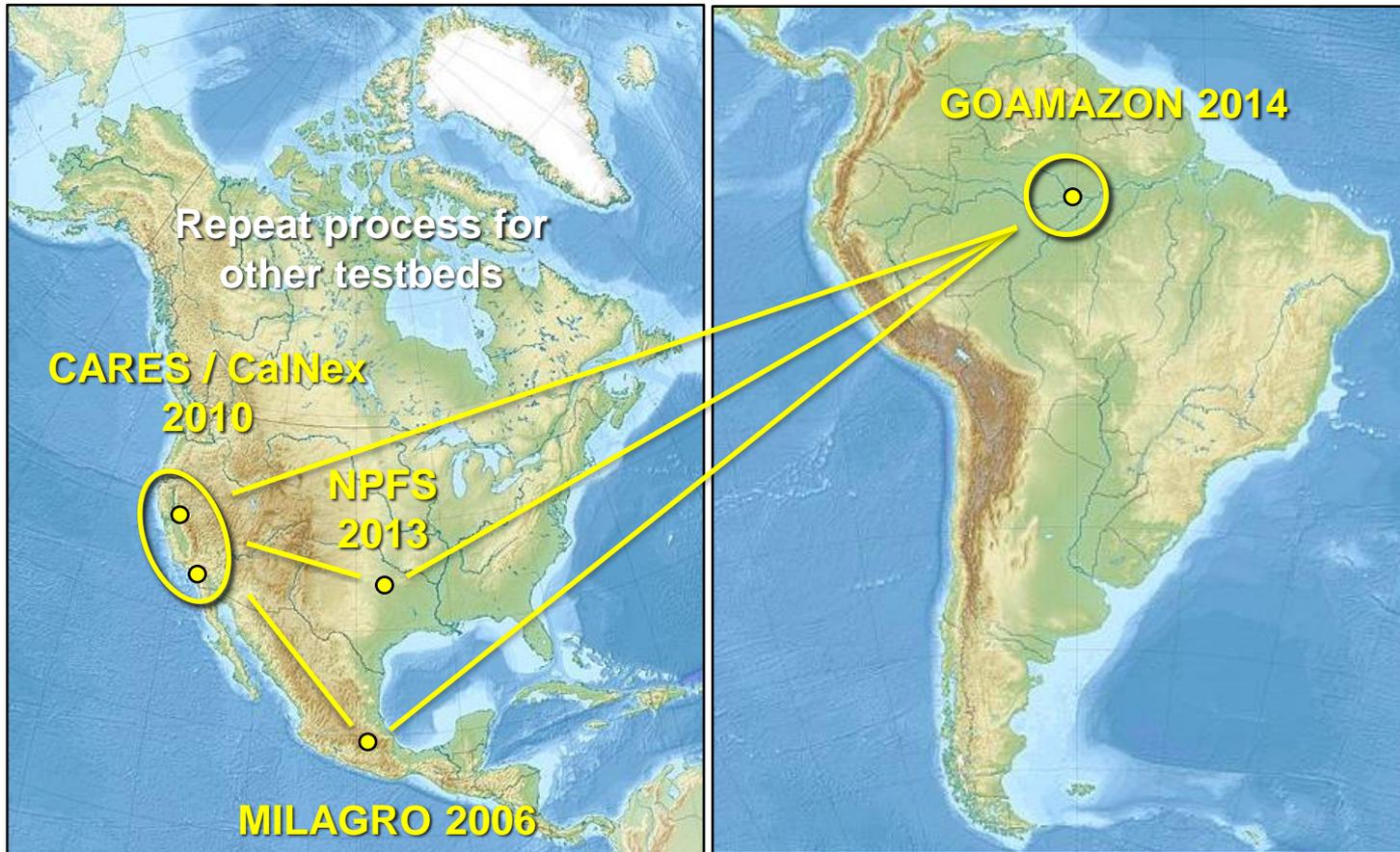
New Particle Formation: One Concept for a Modeling Testbed

A way to organize various activities in the focus group, that ultimately makes an ASR-recommendation of how to better parameterize NPF in climate models based on ARM measurements and ASR science



New Particle Formation: Outcomes from Multiple Testbed Cases

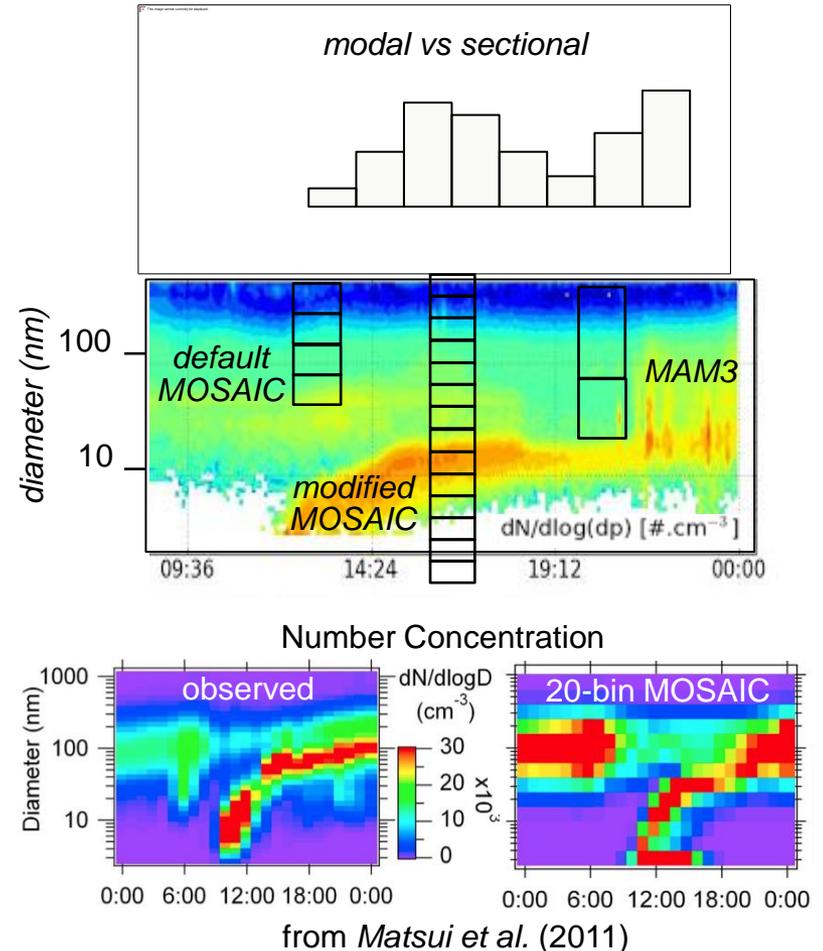
A Long-Term Vision for ASR and the Focus Group



- ▶ Conclusions drawn from performance of a new process module over multiple weather regimes and locales will be more relevant to climate models

New Particle Formation: Modifications / Considerations for Host Model

- ▶ Adapt new process module so that it is compatible with both modal and sectional approaches (software details)
- ▶ MOSAIC would be needed to resolve ultra-fine particles; current 8-bin version range is 40 nm – 10 μm but a 20-bin version available that uses 1 nm to 10 μm
- ▶ Add amine chemistry and emissions or other associated chemistry that lab and field measurements indicate is important
- ▶ Ability to compare performance of a process module with an adequate size distribution (e.g. 20 size bins) with simpler approaches, since climate models not likely to handle the computational expense of complex approaches



from Matsui et al. (2011)
total number concentration from 20-bin version
closer to observed than 8-bin version



Aerosol Mixing State: Potential ARM Datasets for a Testbed Case

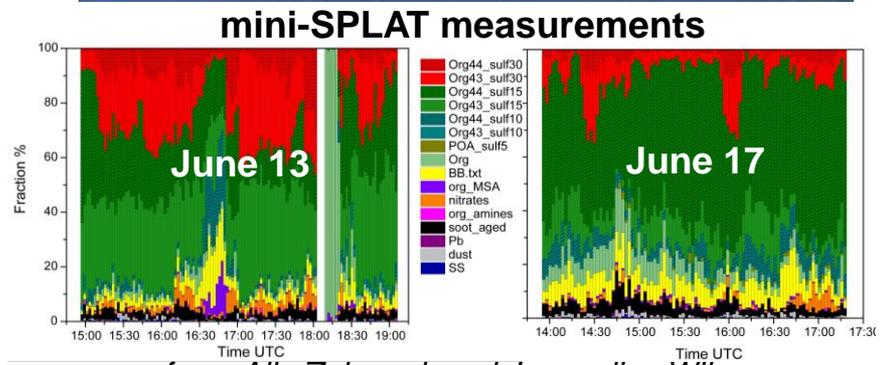
TCAP

- ▶ Cape Cod, July 2012 – June 2013
- ▶ Coincident measurements of single particle data (mini-SPLAT), other aerosol microphysical and optical properties
- ▶ Clean and anthropogenic air masses



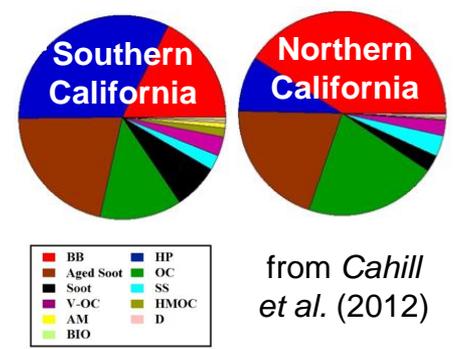
CARES

- ▶ Vicinity of Sacramento, June 2010
- ▶ Coincident measurements of single particle data (SPLAT, ATOFMS, PALMS), scanning microscopy, other aerosol microphysical and optical properties



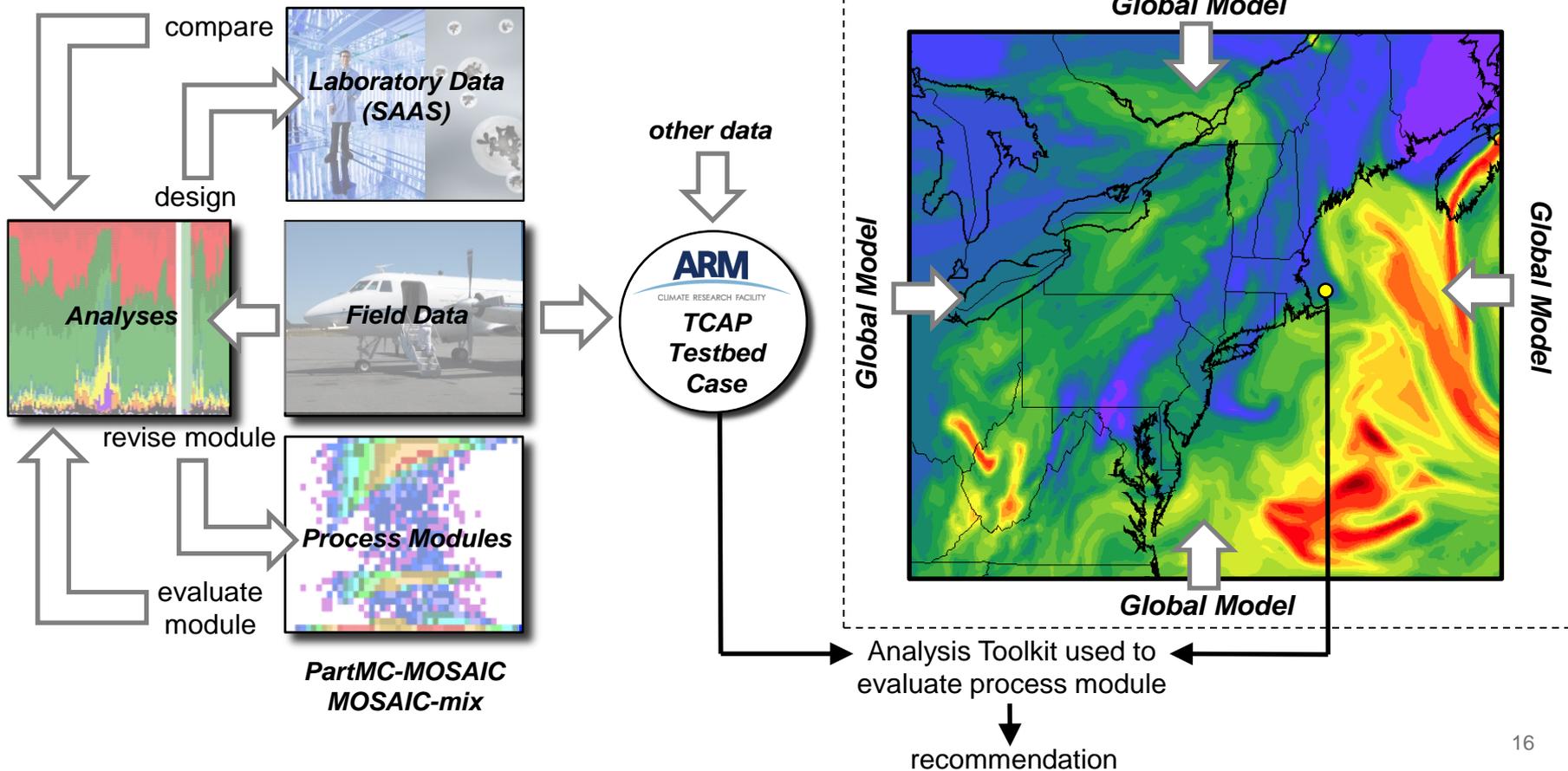
BBOP

- ▶ Smoke from Pacific Northwest forest fires and south-central U.S. agricultural fires, July – October 2013
- ▶ SP2 and SP-AMS measurements



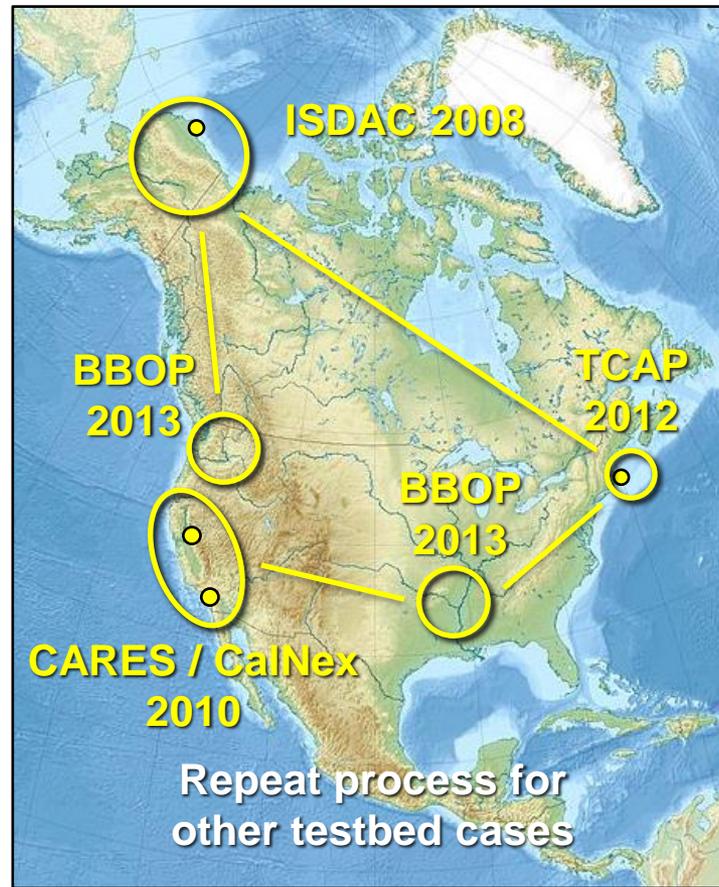
Aerosol Mixing State: One Concept for a Modeling Testbed

A way to organize various activities in the focus group, that ultimately makes an ASR-recommendation of how to better parameterize NPF in climate models based on ARM measurements and ASR science



New Particle Formation: Outcomes from Multiple Testbeds

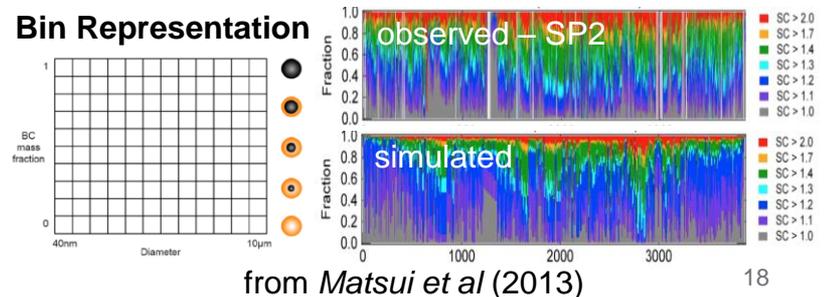
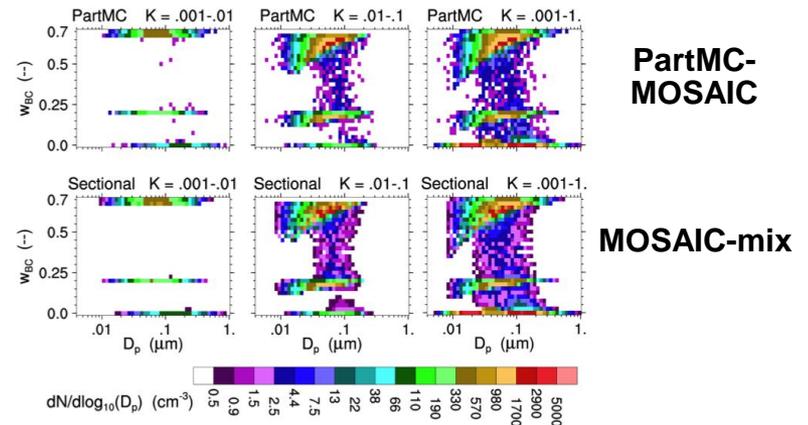
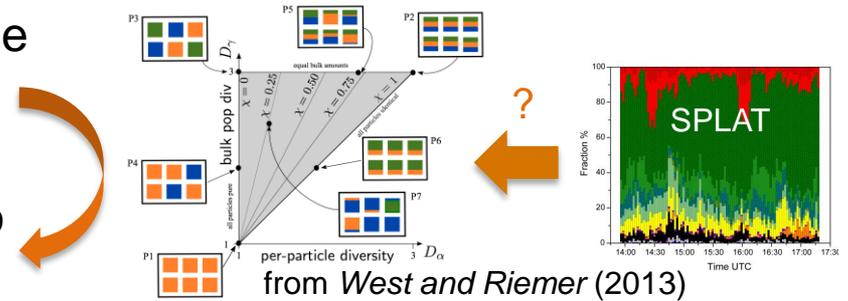
A Long-Term Vision for ASR and the Focus Group



- ▶ Conclusions drawn from performance of a new process module over multiple weather regimes and locales will be more relevant to climate models

Aerosol Mixing State: Modifications / Considerations for Host Model

- ▶ Challenges with interpreting single particle data and how to compare with model representations of aerosols
- ▶ New metrics are needed in the testbed to evaluate 3-D model performance
- ▶ ASR has some box model approaches to represent the evolution of the aerosol mixing state (e.g. PartMC-MOSAIC, MOSAIC-mix), but no modules that could be tested in a regional model
- ▶ Can use present regional model to assess how well internal mixing assumption is when computing optical and CNN properties, but more model development is needed for a 3-D testbed
- ▶ WRF-Chem community has 2 approaches [Matsui et al., 2013, Zhang et al., 2013], but they very computationally expensive



Secondary Organic Aerosol: Potential ARM Datasets for a Testbed Case

CARES / CalNex

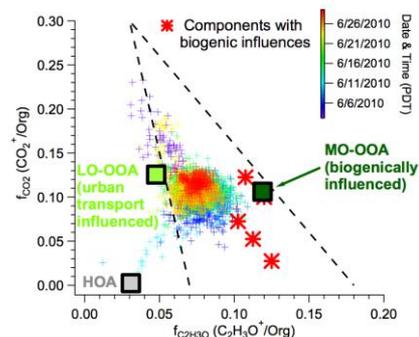
- ▶ California, May - June 2010
- ▶ Extensive ground and airborne data on meteorology, trace gases, and aerosol mass, composition, number, and optical properties
- ▶ Anthropogenic-biogenic interactions

GOAmazon

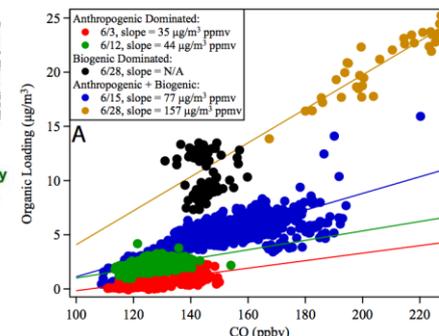
- ▶ Vicinity of Manaus, wet and dry season IOPs 2014
- ▶ Extensive measurements, similar to CARES
- ▶ Both biogenic SOA and anthropogenic-biogenic interactions

Many Other Candidates to Chose From

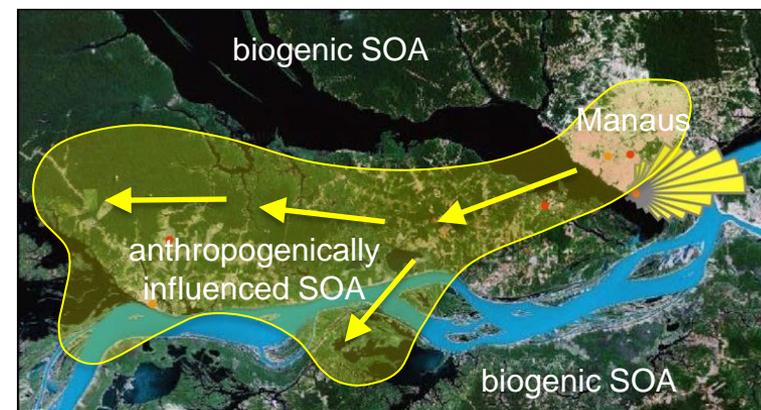
- ▶ Depends on what the focus group wants and can be accomplished in a reasonable time frame (BBOP, TCAP, ClearFO, BNL IOP, MILAGRO)



from Setyan et al. (2012)

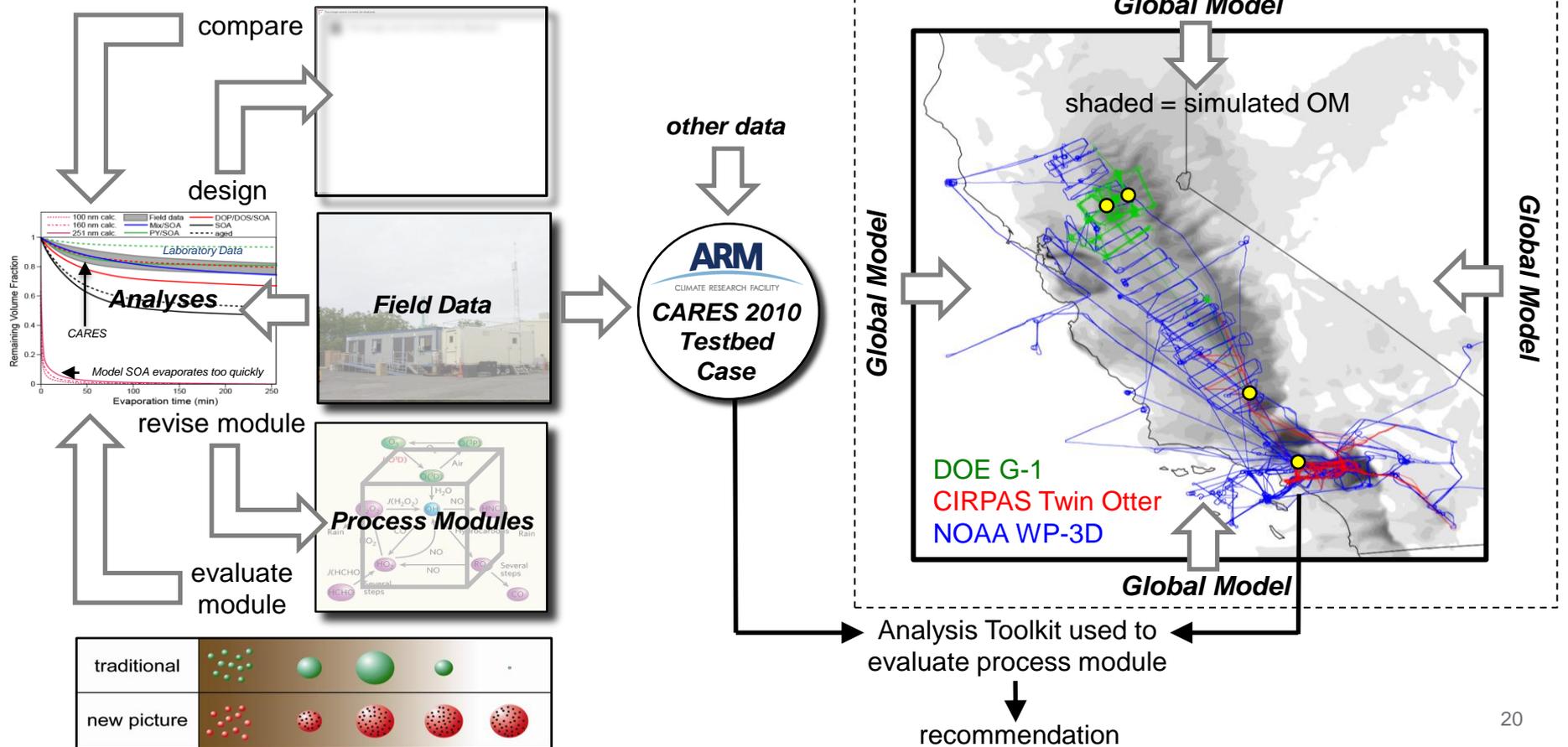


from Shilling et al. (2013)

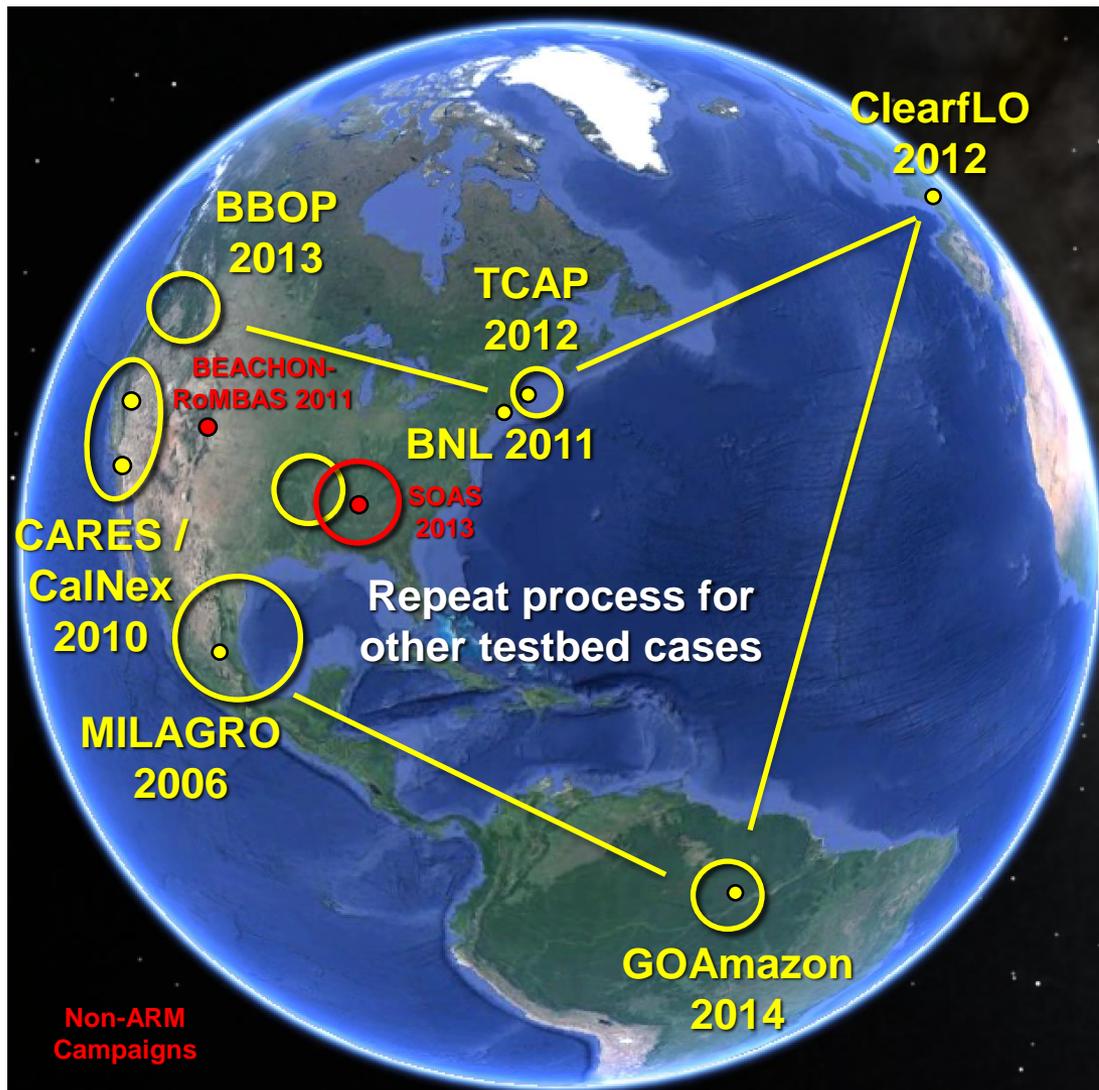


Secondary Organic Aerosol: One Concept for a Modeling Testbed

A way to organize various activities in the focus group, that ultimately makes an ASR-recommendation of how to better parameterize SOA in climate models based on ARM measurements and ASR science



Secondary Organic Aerosols: Outcomes from Multiple Testbed Cases

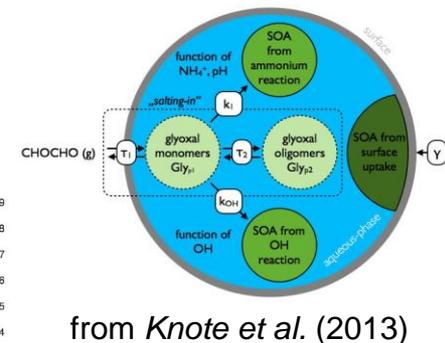
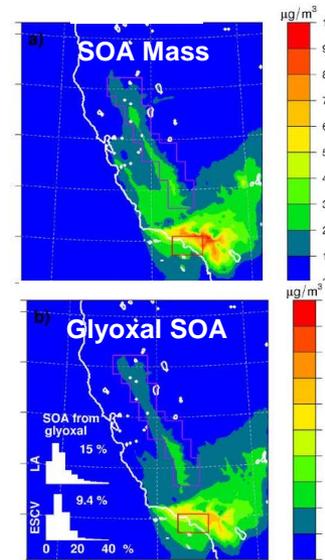
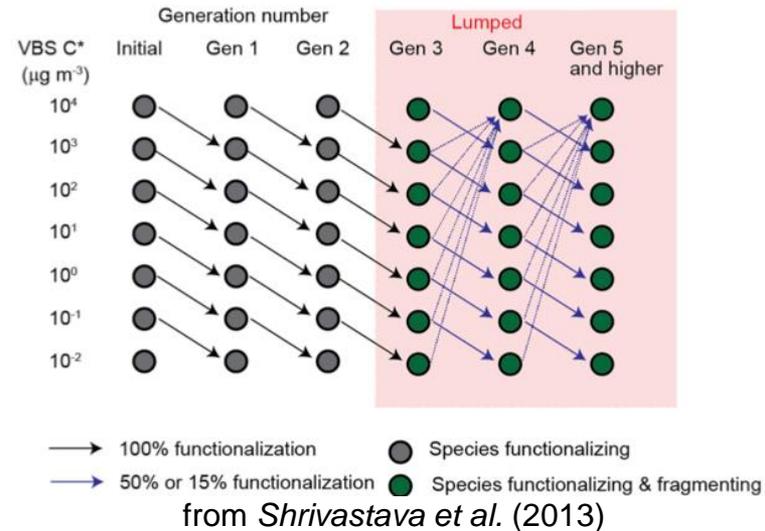


A Long-Term Vision for ASR and the Focus Group

- ▶ The performance of new process modules tested over multiple locales and weather regimes will be more robust and relevant to climate models
- ▶ All cases suitable for OM, but some not suitable to evaluate simulated anthropogenic-biogenic interactions

Secondary Organic Aerosol: Modifications / Considerations for Host Model

- ▶ Much of the work assembling the CARES/CalNex testbed for SOA is complete
- ▶ MOSAIC already has new treatments:
 - VBS that rapidly transforms SOA from semi-volatile to non-volatile particles + gas-phase fragmentation reactions (*Shrivastava et al. 2013*)
 - Glyoxal chemistry coupled with VBS SOA (*Knote et al., 2013*)
- ▶ MAM3 (from CAM5) available ← via SciDAC
- ▶ New more detailed gas-phase mechanism from UK-Manchester available (238 species and 638 reactions) if one wants more detailed hydrocarbon speciation
- ▶ Several WRF-Chem groups (non-ASR) are working on SOA treatments
- ▶ Just need to organize interested modelers and employ AMT methodology to provide more “fair” comparisons



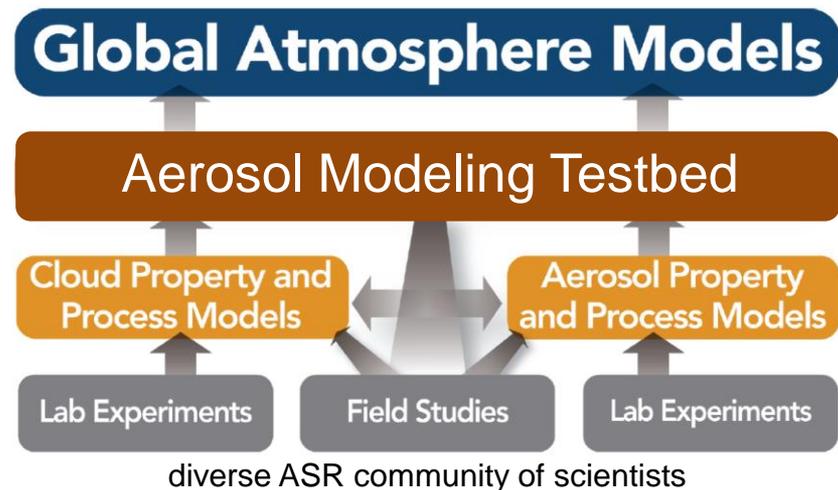
Some of the Challenges

- ▶ Testbed cases are currently being developed under the ARM translator and ASR support, but what is the best way to organize this effort?
 - **Organic approach:** Where scientists naturally work together on problems where there is mutual interest
 - **Top-down approach:** ALWG may want to prioritize which testbeds and aerosol processes should be examined first
 - **Timeframe:** Certain testbeds will be easier to “get off the ground” (e.g. SOA) to produce results than other testbeds (e.g. mixing state).
- ▶ Are there sufficient resources (funding, skills, computing) available within a particular focus group to put together parts of a testbed that is not being addressed by current activities?
- ▶ How do we deal with logistical considerations when working in a group, especially those associated with different funding cycles and schedules?
- ▶ Are there other testbeds on other aerosol processes (with or without interactions with clouds) with sufficient interest from ASR investigators?
- ▶ Are scientists concerned about working in groups where “proprietary” knowledge may leak out?

*both take time
and effort to
organize*

- ▶ A **vision** of how the aerosol modeling testbed could be used to address objectives of the ASR Aerosol Lifecycle focus groups is presented
 - The methodology can be extended and applied to address the objectives of CAPI and CLWG as well
- ▶ More details on the focus groups, ARM field measurements, and lab studies will be presented in the **breakout sessions to follow** ...

- ▶ So there should be more opportunity to discuss how testbeds can fit into focus group activities as well as how they can be used to organize ARM data and ASR science in a **measurements-to-modeling approach**



from ASR
Science Plan

- ▶ For those interested in more details, the August CESD Atmospheric Testbeds Workshop will be summarized and discussed in a cross-WG breakout session **Wednesday night**



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Questions?