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An Efficient Representation of Aerosol Mixing State for Atmospheric Models

Joseph Ching[1], Rahul Zaveri[1], Richard Easter[1], Alla Zelenyuk[1], Jerome Fast[1]
Nicole Riemer[2], R. Subramanian[3], Art Sedlacek[4]

[1]Pacific Northwest National Laboratory, Richland, WA, USA
[2]University of Illinois at Urbana-Champaign, Urbana, IL, USA
[3]Carnegie Mellon University, Pittsburgh, PA, USA
[4]Brookhaven National Laboratory, Upton, NY, USA

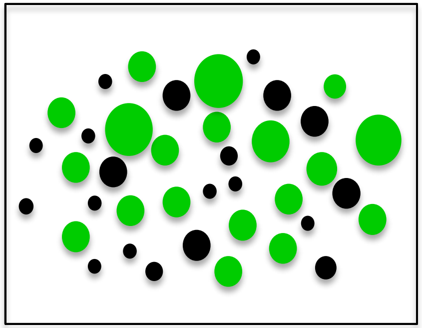
3.13.2017 - 3.16.2017
DOE ARM/ASR PI meeting

ASR Atmospheric System Research

U.S. DEPARTMENT OF ENERGY

What is aerosol mixing state?

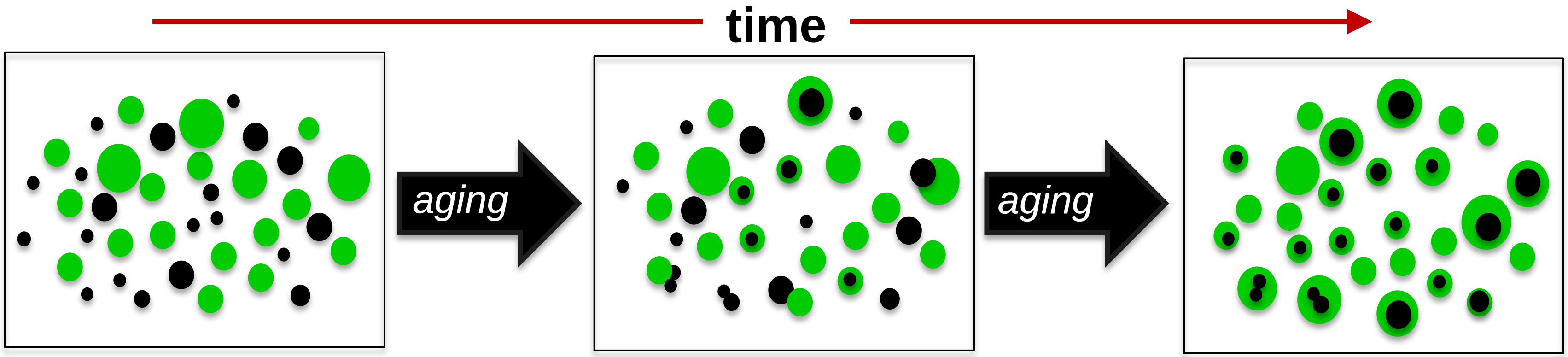
Aerosol mixing state:
distribution of per-particle chemical species composition. [*Riemer and West 2013*]



externally mixed population

What is aerosol mixing state?

Aerosol mixing state:
distribution of per-particle chemical species composition. [*Riemer and West 2013*]

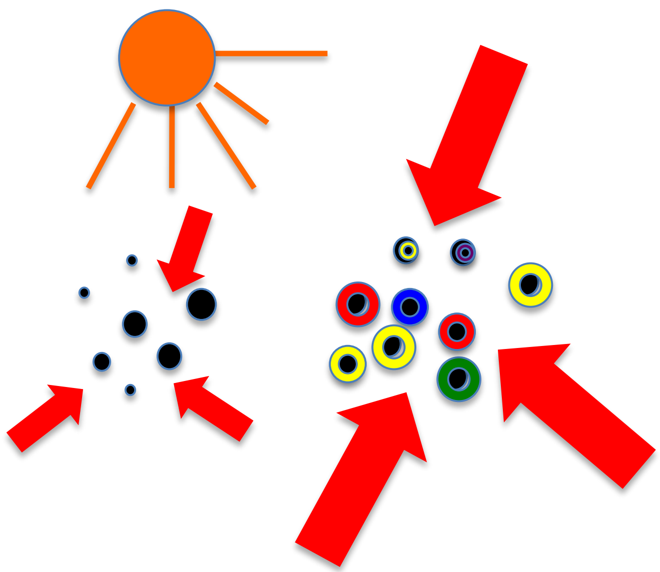


externally mixed population

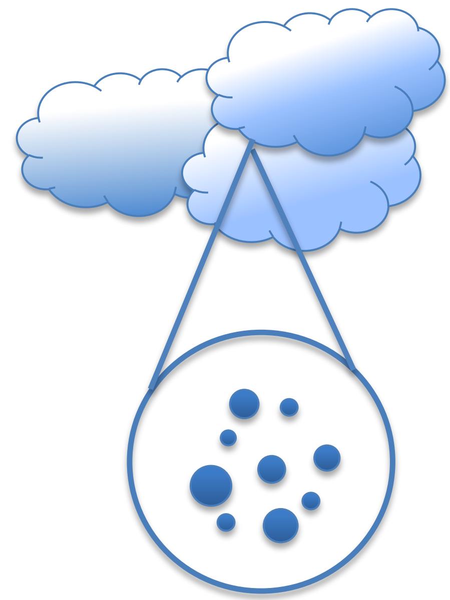
intermediate mixing

more internally mixed population

Climate relevancy of aerosol mixing state



Absorption enhancement



Acting as CCN

Both CCN and optical properties depend on *size and mixing state*.

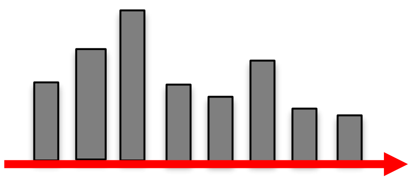
Objective

To reliably predict *CCN and optical properties* as a function of size and mixing state at a *reasonable computational cost*

- Develop a novel sectional framework to resolve aerosol mixing state: MOSAIC-mix.
- Apply the model using single particle measurements (SPLAT-II and SP2) during CARES to simulate aerosol mixing state evolution.

MOSAIC-mix sectional framework

MOSAIC:
Sectional approach resolving size only



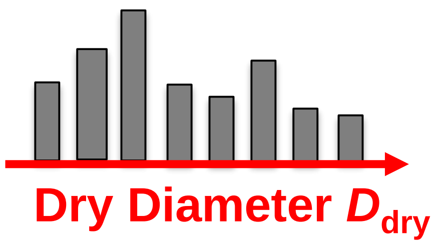
Dry Diameter D_{dry}

In each size bin,
all particles have
same BC mass fraction w_{BC}
and
same hygroscopicity (κ)

Zaveri et al. (2008)
MOdel for **S**imulating **A**erosol **I**nteractions and **C**hemistry

MOSAIC-mix sectional framework

MOSAIC:
Sectional approach resolving size only



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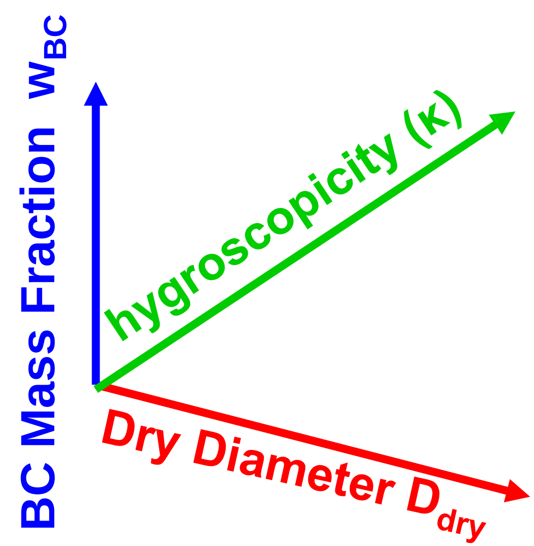
Zaveri et al. (2008)

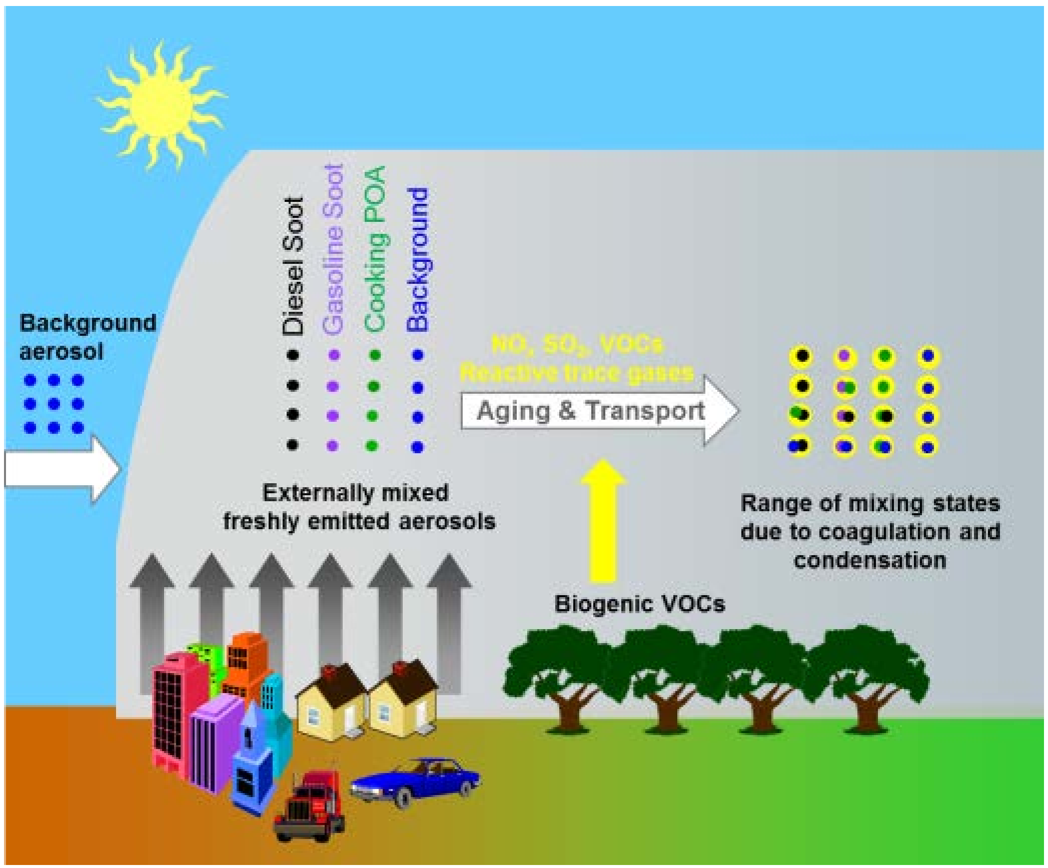
MOSAIC-Mix:
Resolves size, BC mass fraction and hygroscopicity



Ching et al. (2016)

Approach

- Use 10 idealized urban scenarios to simulate aerosol mixing state evolution under different emissions and environmental conditions.
- Optimize the sectional framework using a high-resolution version of MOSAIC-mix and particle-resolved model PartMC-MOSAIC [*Riemer et al*. 2009].



10 Urban Plume Scenarios

- Gaseous emissions
- Black carbon emission
- Background particle concentration
- Solar radiation
- Temperature
- Relative humidity

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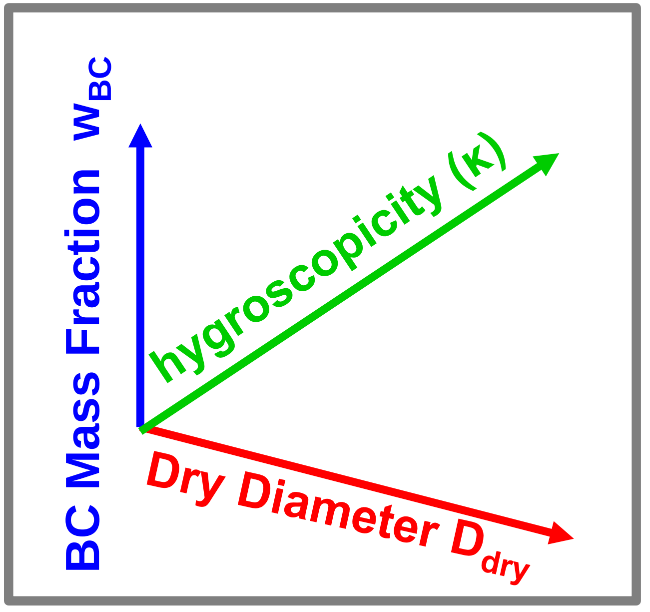
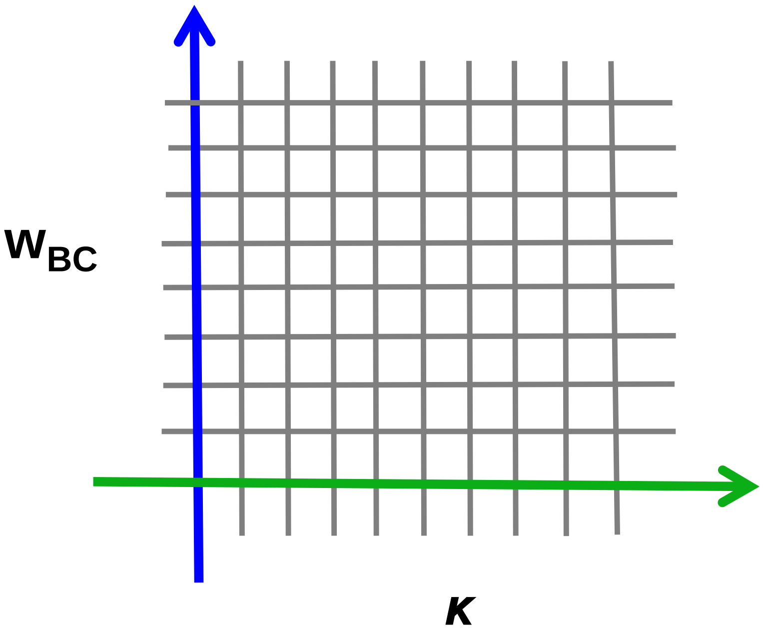
Approach





- High-resolution MOSAIC-mix with **24 D_{dry} x 35 w_{BC} x 30 κ**

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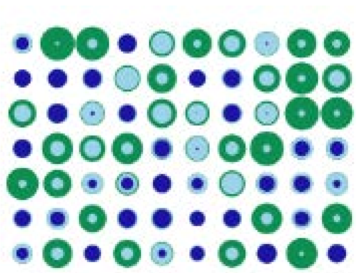
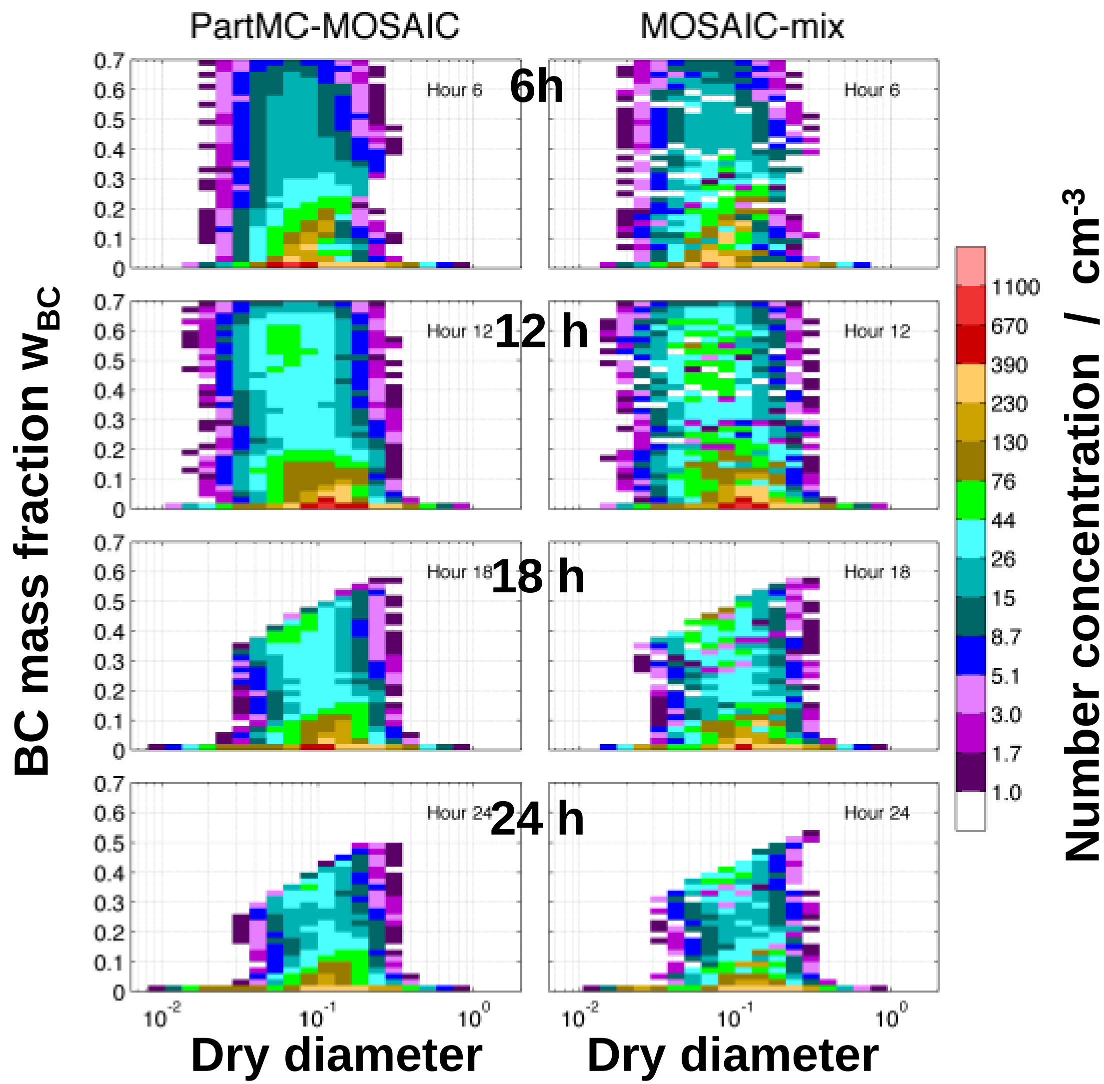
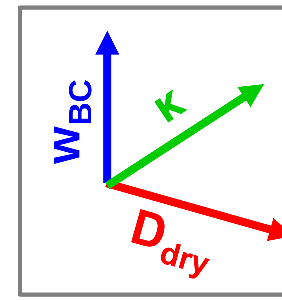
Benchmarking

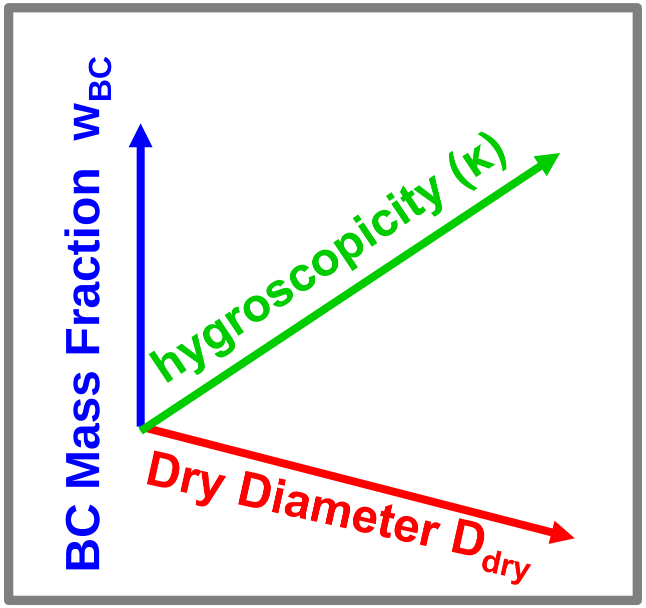
- High resolution MOSAIC-mix was evaluated against particle-resolved model PartMC-MOSAIC.

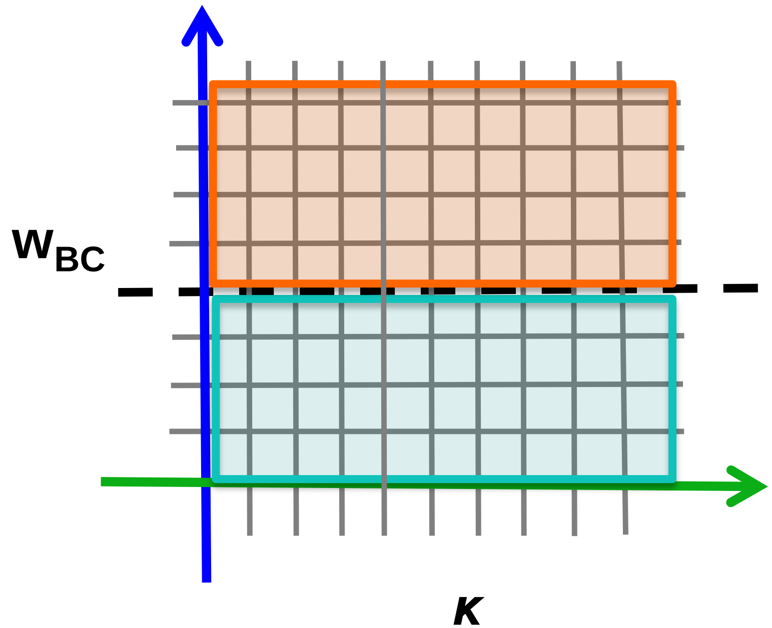






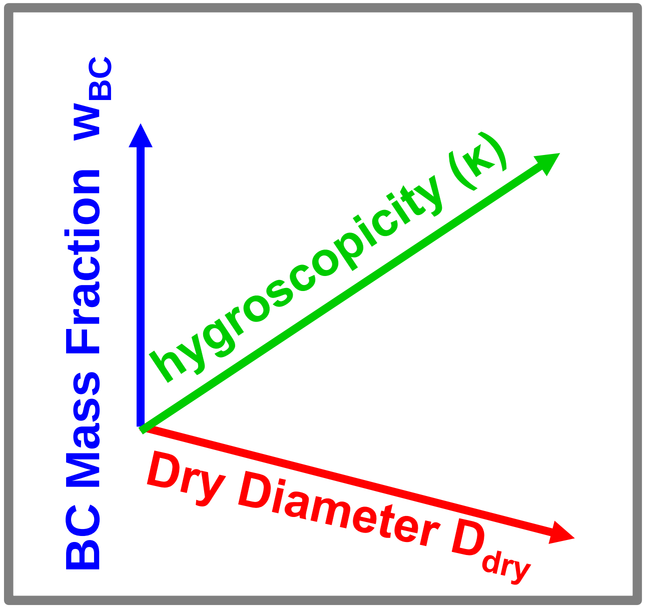
Approach

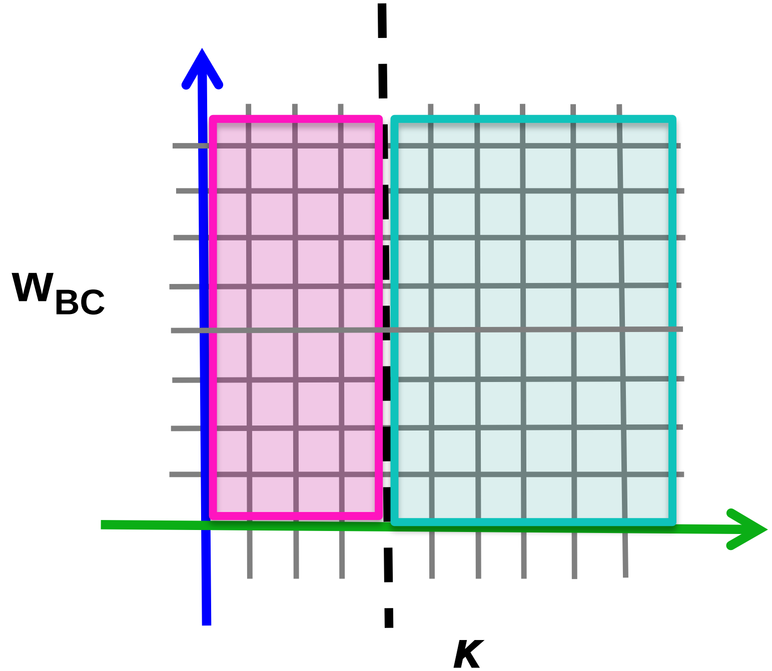




- Devise low-resolution MOSAIC-mix

Approach





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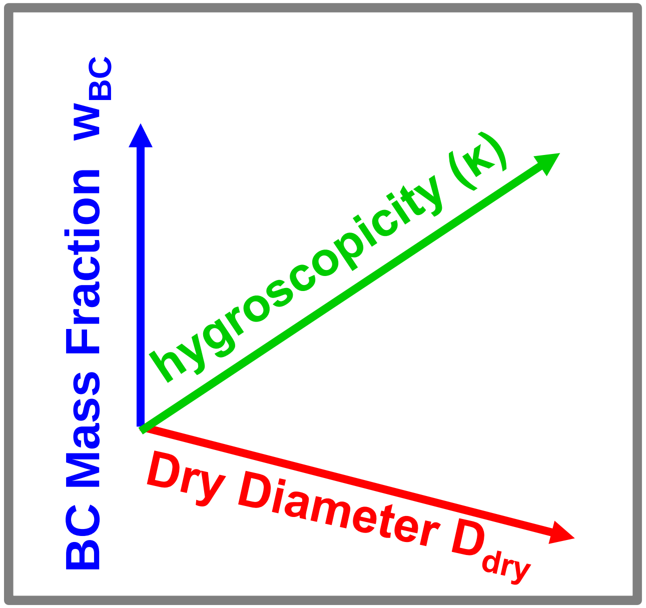
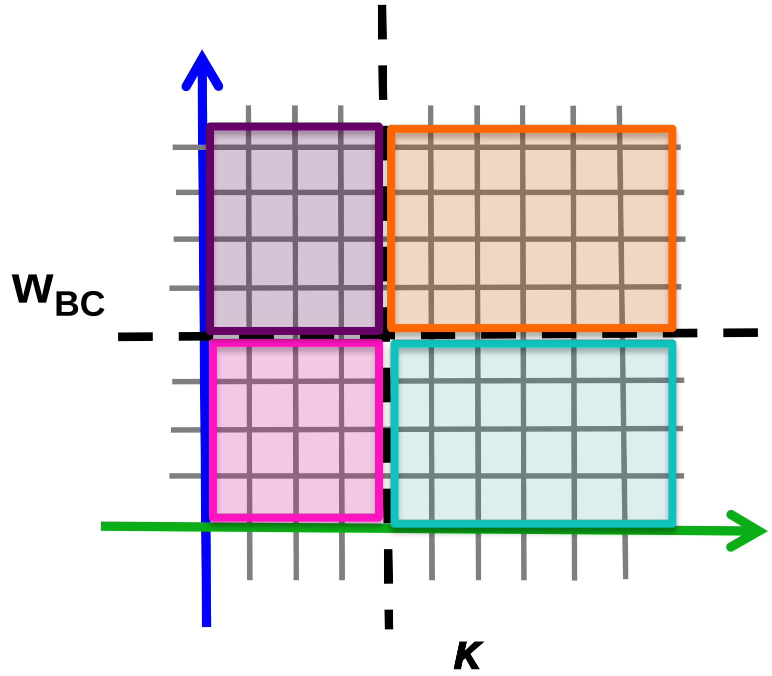
Approach





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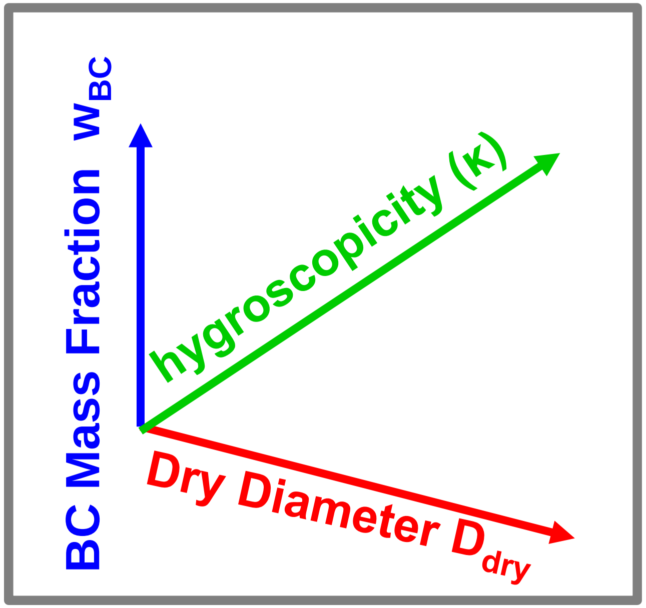
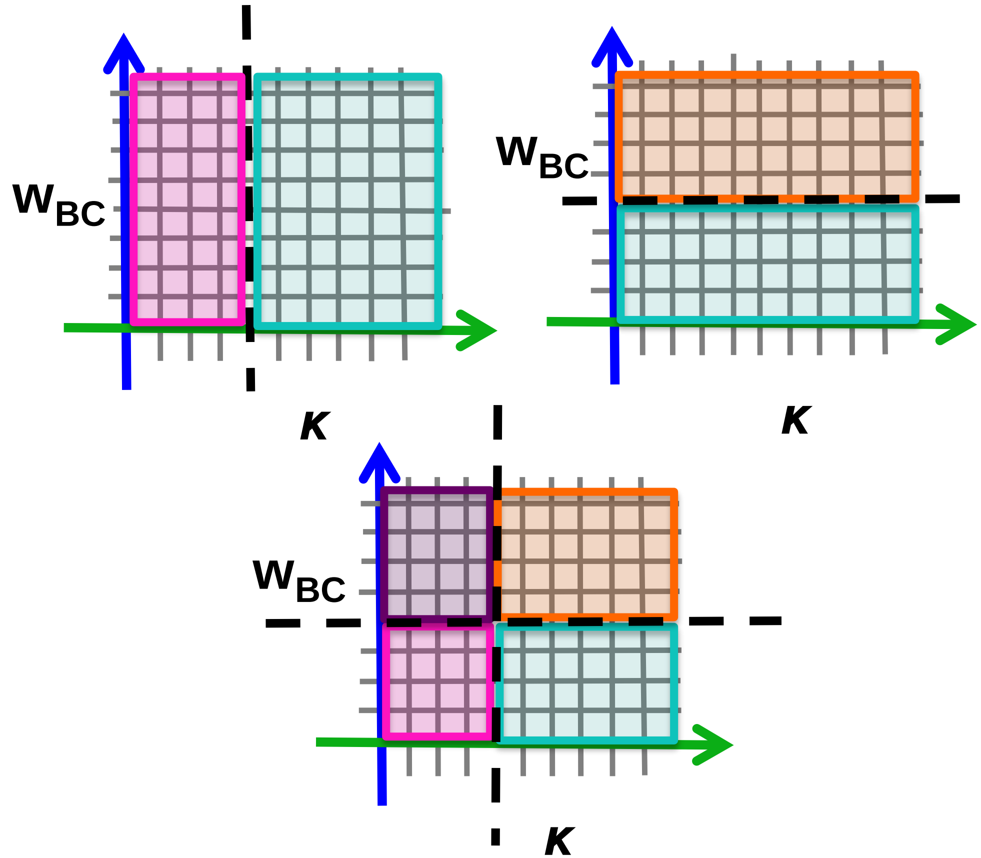
Approach

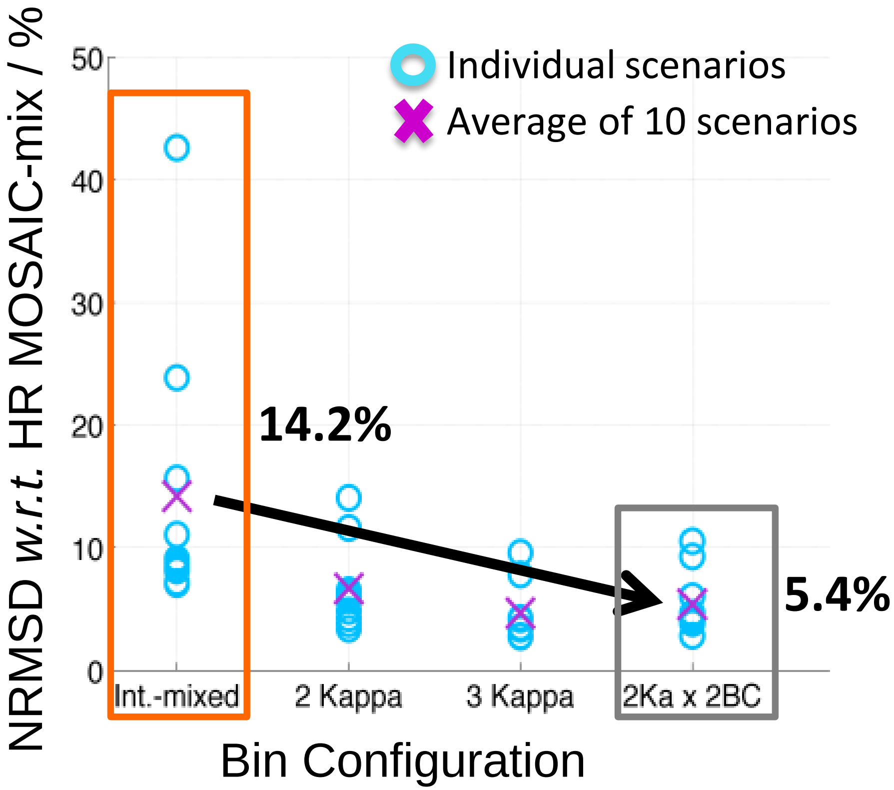


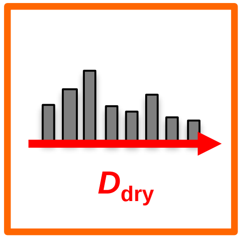


- About 2,000 low-resolution configurations in 1D, 2D, or 3D (**24 D_{dry} x 1-3 w_{BC} x 1-3 κ**) with different choices of bin boundaries evaluated against the high-resolution configuration.

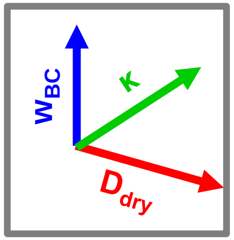
Performance

CCN concentrations





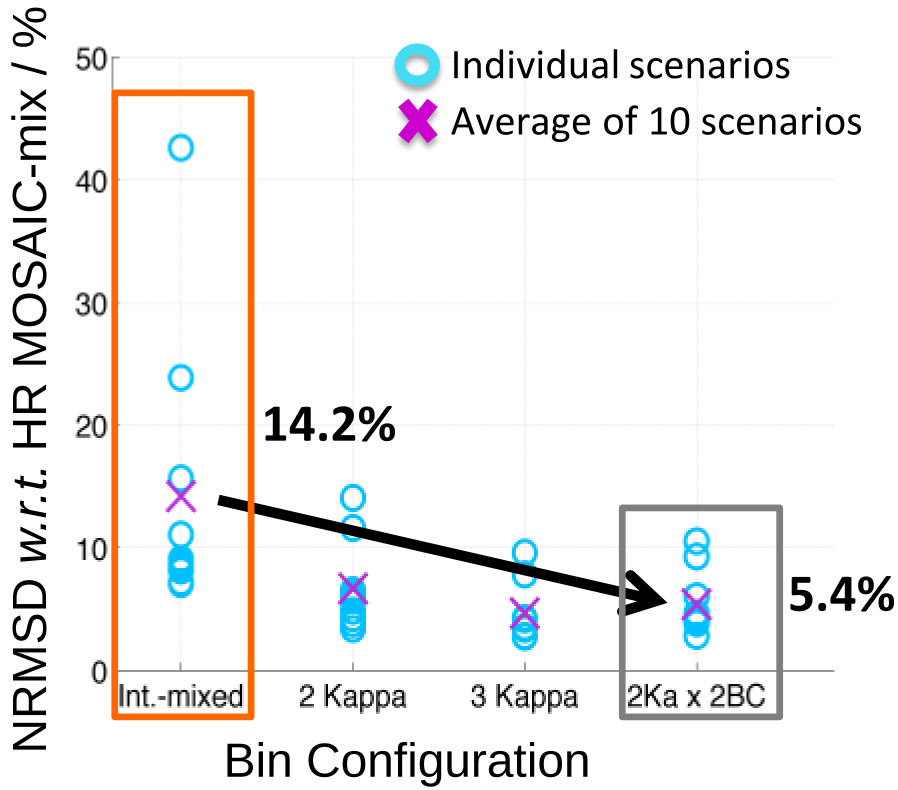
Internally mixed
(24 x 1 x 1)



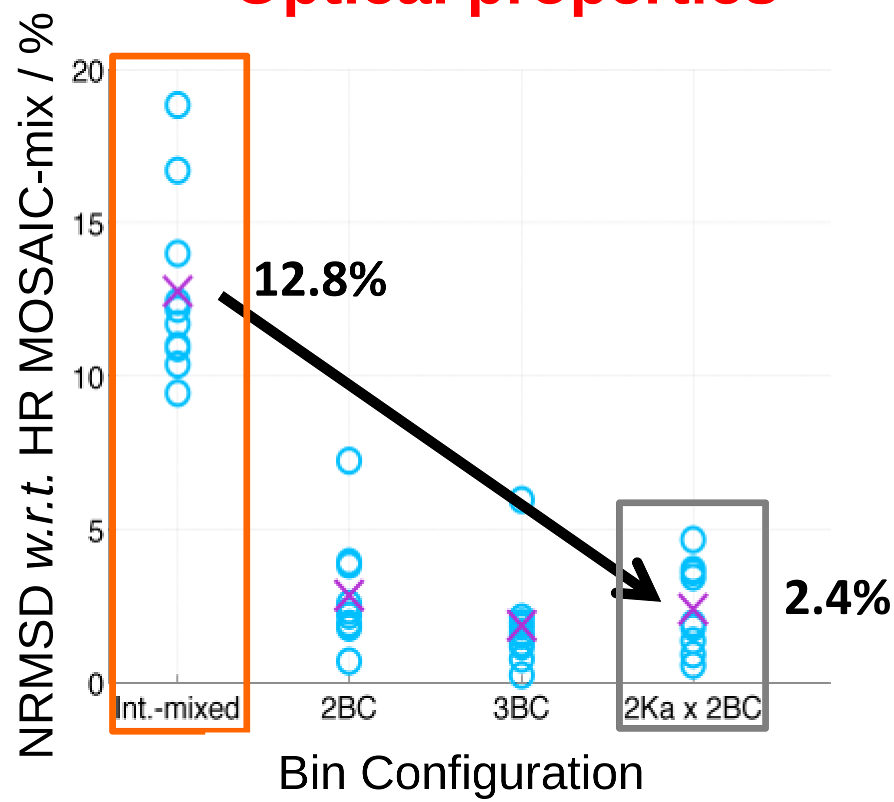
(24 x 2 x 2)

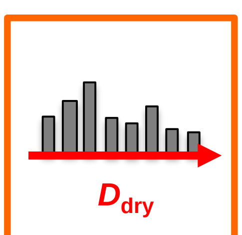
Performance

CCN concentrations



Optical properties





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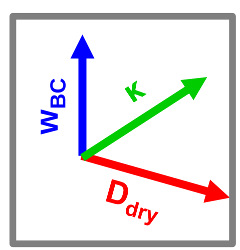


(24 x 2 x 2)

CARES campaign

June 2 – 28, 2010

Zaveri et al. ACP 2012

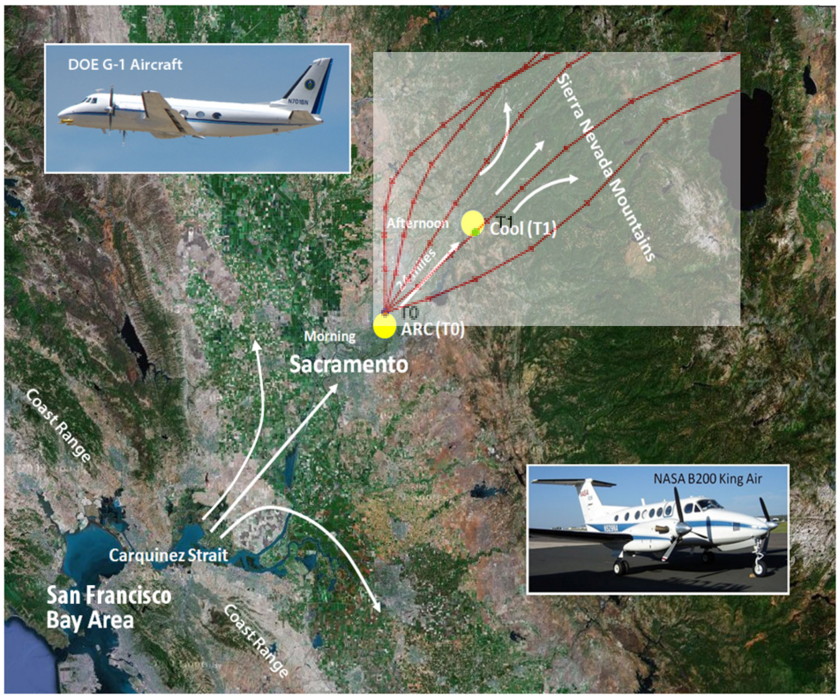
CARES Objectives:

- Investigate Anthropogenic-Biogenic Interactions in SOA formation.
- Investigate black carbon (BC) mixing state evolution.
- Quantify the effects of aerosol ageing on aerosol optical and CCN activation properties.

Lagrangian simulations by MOSAIC-mix and PartMC-MOSAIC

ARM
CLIMATE RESEARCH FACILITY

June 2 – 28, 2010



Zaveri et al. ACP 2012

- Used **5 trajectories** originating from T0 on June 15 from a FLEXPART-WRF simulations Fast et al. (2012).
- **Same gas and aerosol emission, initial and background conditions** were input to both PartMC-MOSAIC and MOSAIC-mix
- Model simulations were **compared to G-1 observations**

Model initialization using single particle measurements at T0

To derive initial conditions for model simulations, we used

- SMPS and APS - size distributions
- SPLAT–II - size and mixing state distributions of non-BC containing particles
- SP2 – size and mixing state distributions of BC-containing particles

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Deriving BC size and mixing state distribution from SP2

Assumed: Spherical shape
Core-shell structure

Total diameter: $D_{total} = D_{core} + D_{coat} \times 2$

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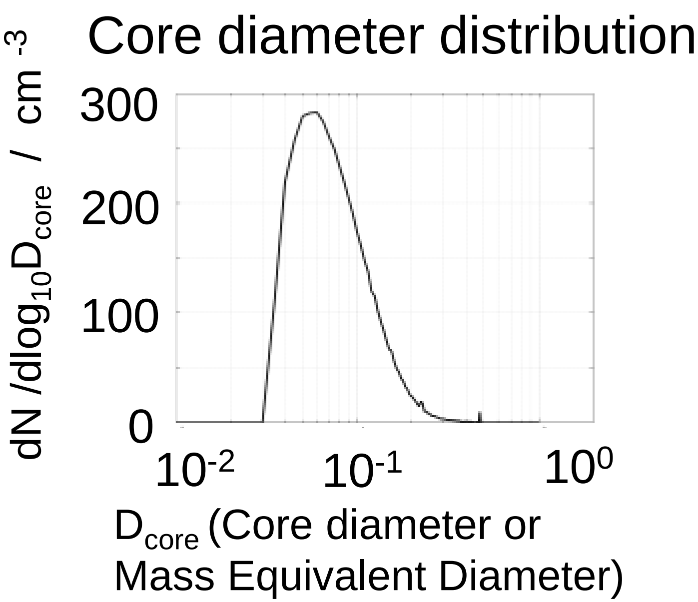

Deriving BC size and mixing state distribution from SP2

Assumed: Spherical shape
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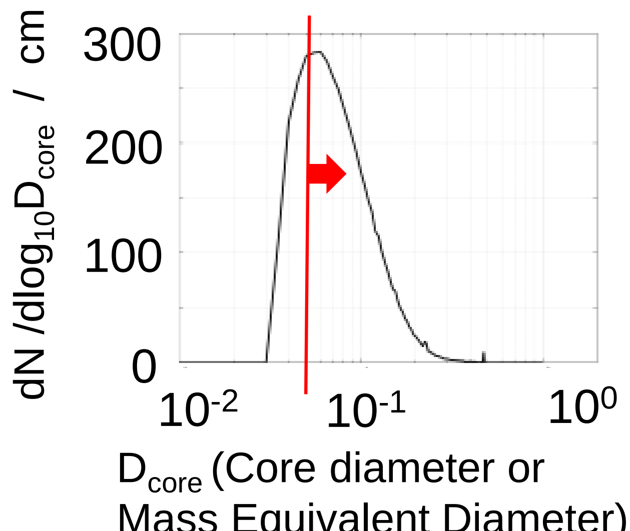
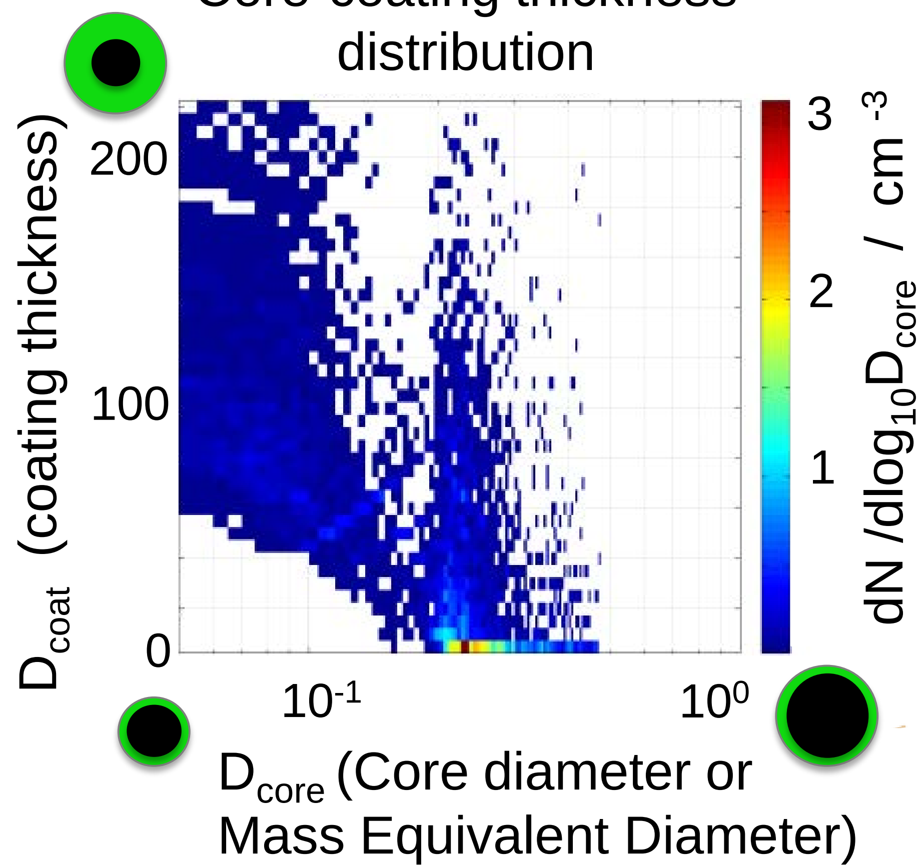
Total diameter: $D_{total} = D_{core} + D_{coat} \times 2$

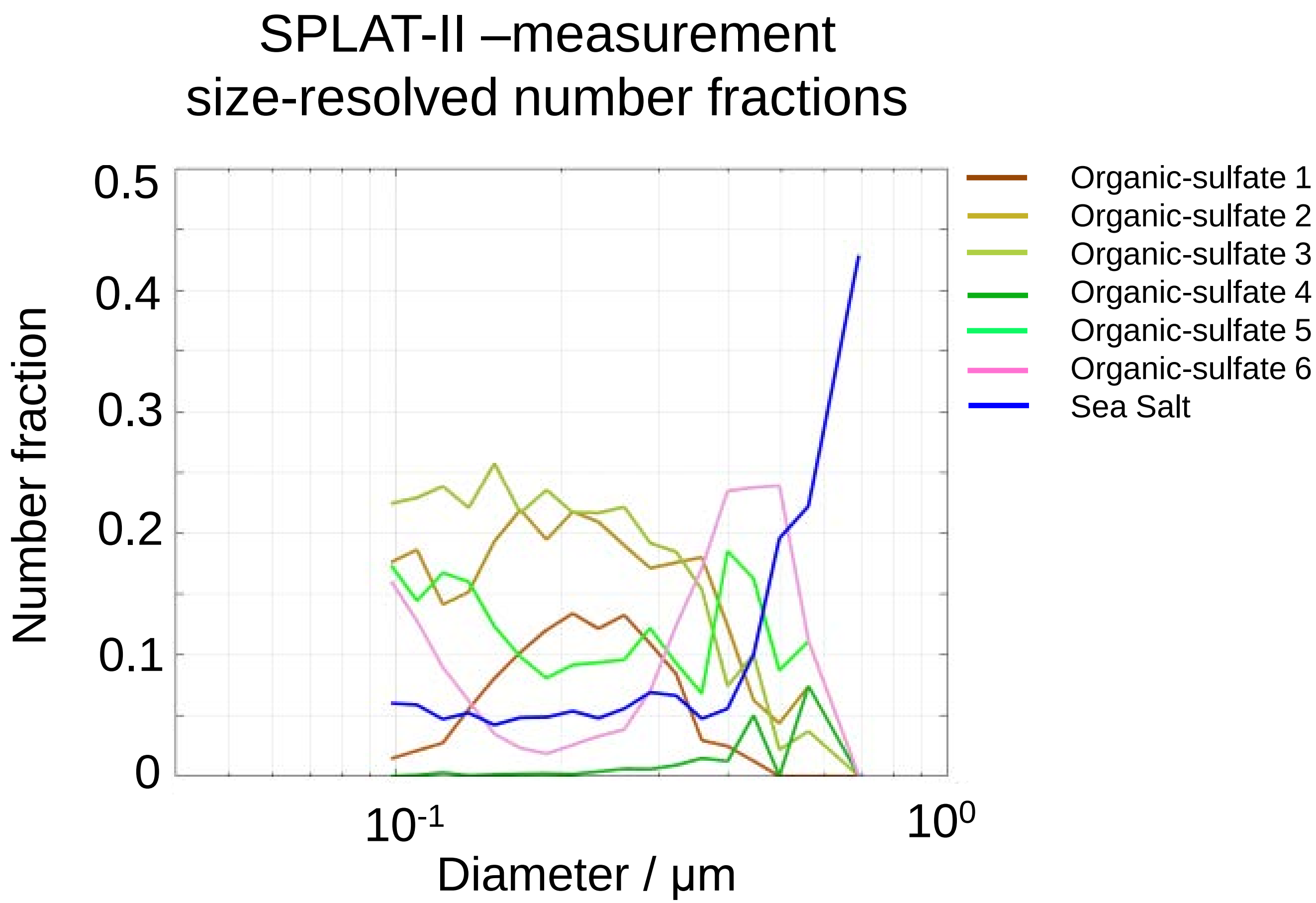
Core diameter distribution



Core-coating thickness distribution



Deriving size and mixing state distribution from SPLAT- II



We consider 7 particle classes from SPLAT, ***6 organic-sulfate and sea salt***.

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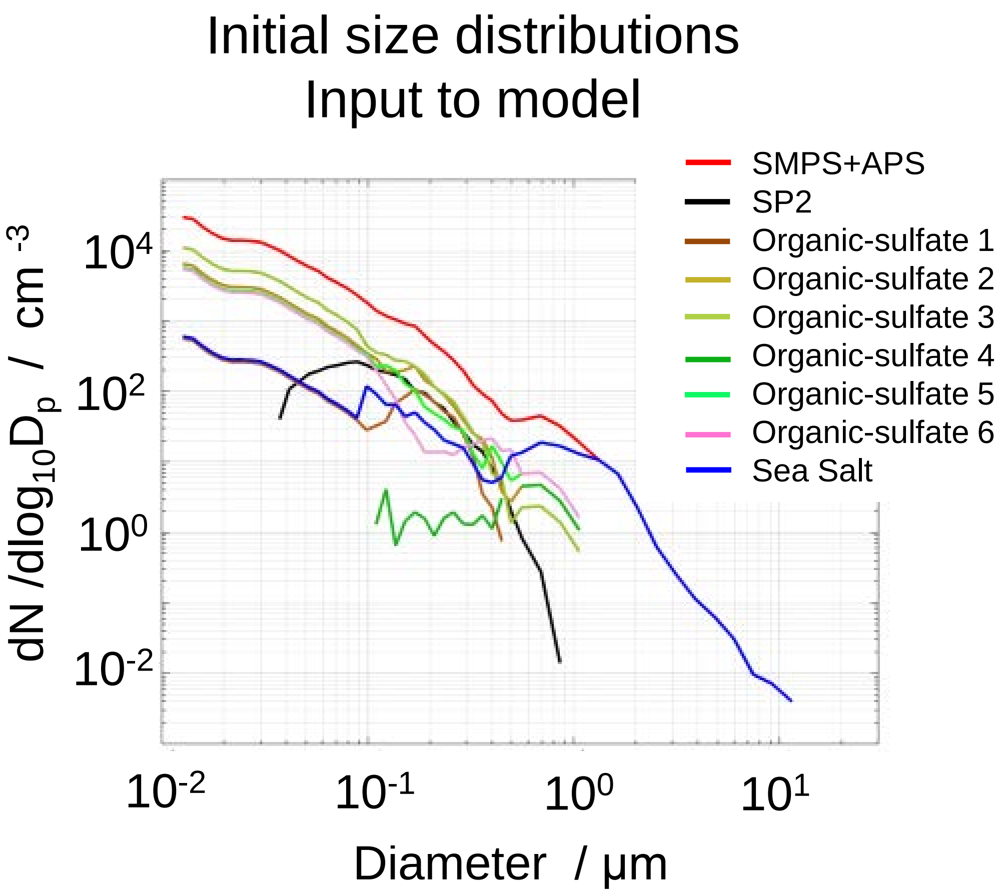
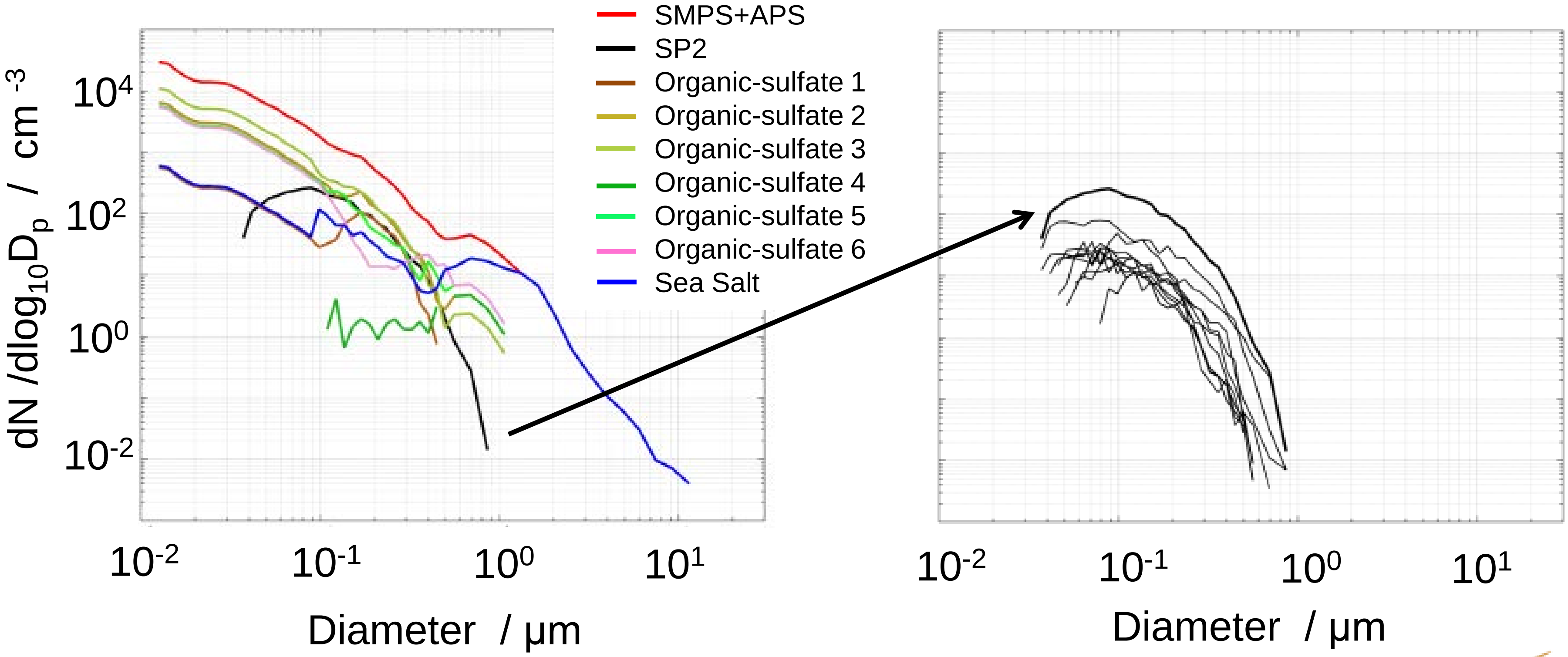
Deriving size and mixing state distribution from SPLAT- II and SP2



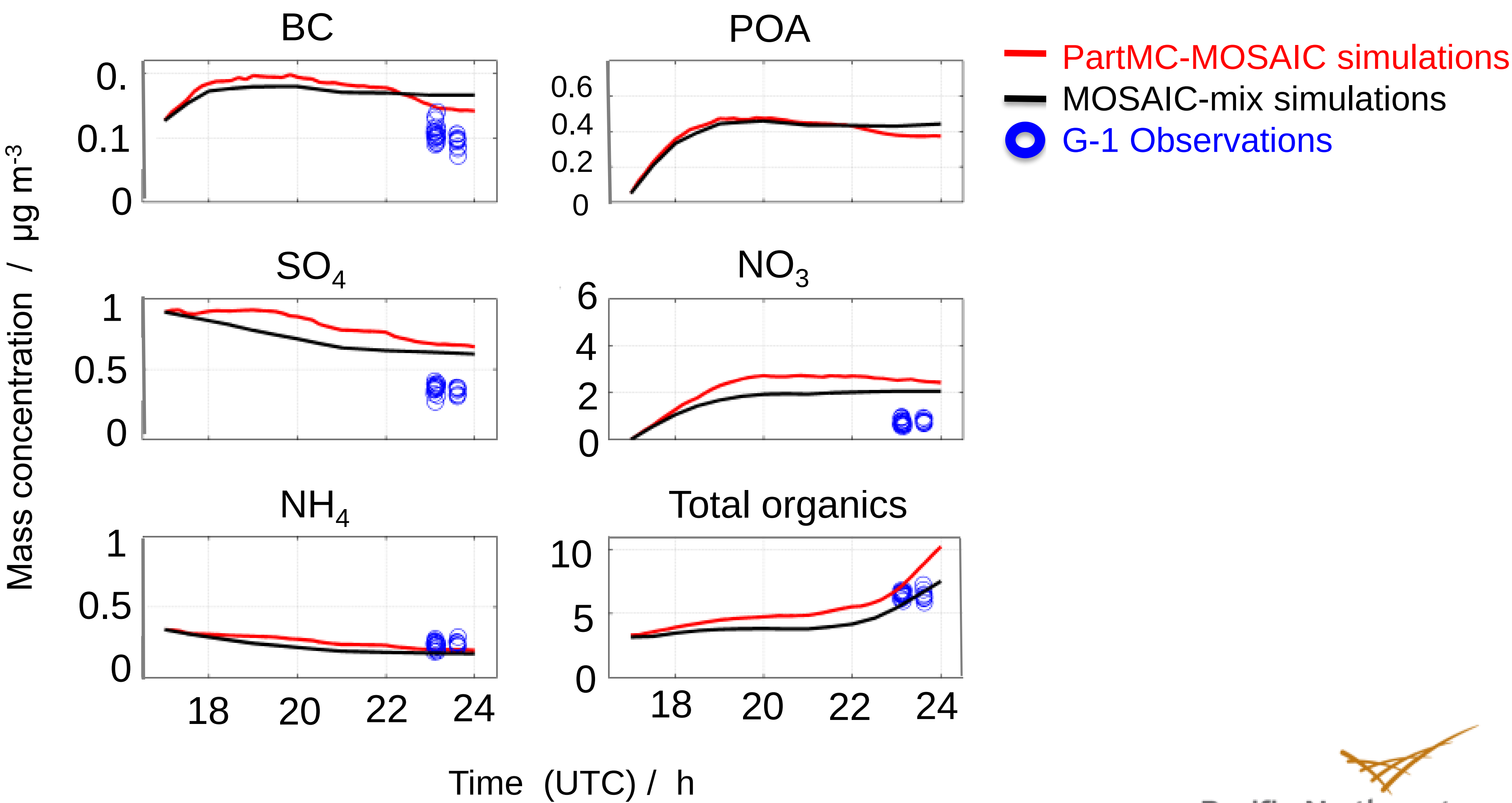
Deriving size and mixing state distribution from SPLAT- II and SP2

Initial size distributions
Input to model

10 Initial size distributions input to the model ***derived from SP2***



Aerosol mass concentrations simulations vs G-1 observations



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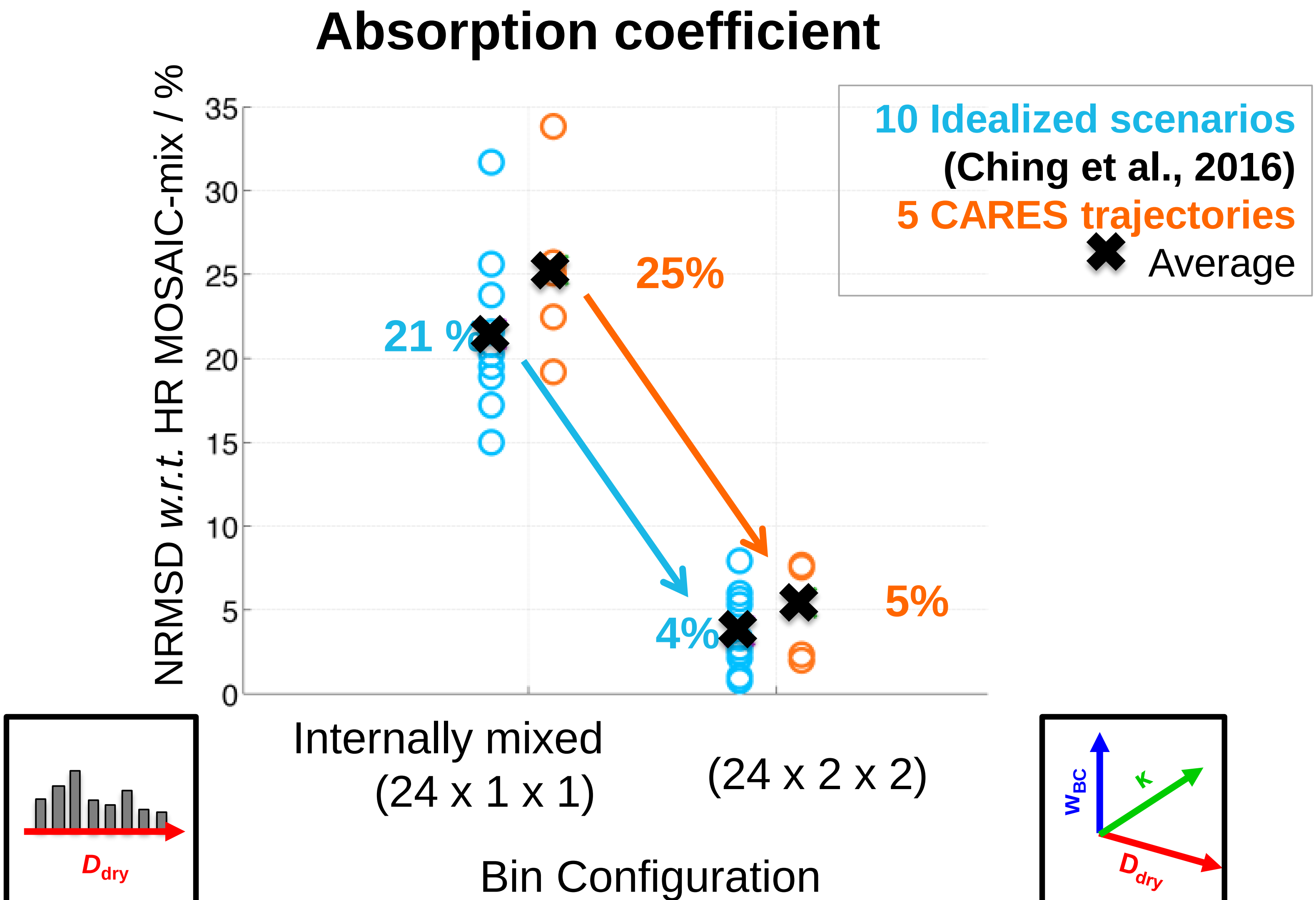
Size-resolved vs mixing-state-resolved



Summary

- Developed *a novel sectional framework that efficiently resolves mixing state: MOSAIC-mix*.

- Showed that *mixing-state-resolved* simulations better predict the CCN and optical properties than size-resolved only simulations with a *small number of mixing state bins*.

- Applied the model using *initial conditions* from SPLAT-II and SP2 *single particle measurements* during CARES.

- MOSAIC-mix is being implemented in WRF-Chem to assess the impacts of aerosol mixing state at regional scale.

For more details, please refer to poster *71*.