Mixing State Focus Group

Mixing state definition:

- **Population mixing state:** the distribution of chemical compounds across the particle population,

- **Morphological mixing state**: the distribution of chemical compounds within and on the surface of each particle.

Scientific Questions

- Q1: What is the impact of mixing state on the climate-relevant properties of aerosol particles?
- Q2: What mixing state information should be included in models that quantify aerosol climate impacts?
- Q3: What mixing state information should be measured in the field and in the lab?
- Q4: How can we connect measurements (lab and field) to each other and to modeled mixing state information?

Table 1:
Mixing State and Climate-Relevant Properties

Quantities	LOSU	PRM	RM	GCM	Comments
CCN concentration	high	fair	poor	poor	Good parameterizations available on the microscale (e.g., kappa model). Significant amounts of lab and field data available.
Optical properties	med	fair	poor	poor	Excellent models available assuming spherical particles and Mie theory. Poor understanding of morphology effects.
IN concentration	low	poor	poor	poor	Conflicting experimental data. No consensus on correct modeling approach.

Table 1: Climate relevant quantities that depend on aerosol mixing state, our level of scientific understanding (LOSU) of the basic physics involved in describing mixing state effects, and our ability to represent these mixing state effects in particle-resolved models (PRM), regional models (RM), and general circulation models (GCM).

Table 2:
Connections between Different Tools

	Theory/ Metrics[1]	PRM[2]	GCM[3]	SP2[4]	Micros-copy[5]	SP mass spectro-metry[6]	Remote sensing[7]	Bulk measure-ments[8]
Theory/ Metrics[1]		high	low	medium	medium	low	low	low
PRM[2]	high		low	medium	low	low	low	high
GCM[3]	low	low		low	low	low	high	medium
SP2[4]	medium	medium	low		low	low	low	high
Micros-copy[5]	medium	low	low	low		low	low	medium
SP mass spetro-metry[6]	low	low	low	low	low		low	medium
Remote sensing[7]	low	low	high	low	low	low		high
Bulk measure-ments[8]	low	high	medium	high	medium	medium	high	

Table 2: Assessment of current abilities to connect data and outputs amongst different tools. The lack of comparable mixing state outputs between many tools is a key bottleneck in our ability to understand mixing state impacts.

Bottleneck:

Lack of comparable mixing state outputs between many tools

Table 2: Connections between Different Tools

	Theory/ Metrics[1]	PRM[2]	GCM[3]	SP2[4]	Micros-copy[5]	SP mass spectro-metry[6]	Remote sensing[7]	Bulk measure-ments[8]
Theory/ Metrics[1]		high	low	medium	medium	low	low	low
PRM[2]	high		low	medium	low	low	low	high
GCM[3]	low	low		low	low	low	high	medium
SP2[4]	medium	medium	low		low	low	low	high
Micros-copy[5]	medium	low	low	low		low	low	medium
SP mass	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]		[illegible]	[illegible]

Bottleneck:

Lack of comparable mixing state outputs between many tools

How can we improve the connections between poorly-connected tools?

Table 2: Assessment of current abilities to connect data and outputs amongst different tools. The lack of comparable mixing state outputs between many tools is a key bottleneck in our ability to understand mixing state impacts.

Table 3: Readiness of Tools

	Population mixing state		Morphological mixing state	
	Readiness level	Deliverables	Readiness level	Deliverables
Theory/Metrics	high	D1, D6, D9	low	D9
PRM	high	D2, D6, D8, D10, D11, D13	low	D11
RM	low	D4, D7, D13	low	
GCM	low	D3, D4, D13	low	
SP2	medium	D5, D6, D8, D10, D12	medium	D6, D10
Microscopy	medium	D1, D8, D12	high	D6, D5
Single-particle mass spetrometry	high	D8, D12	low	

Table 3: Readiness of tools to represent population mixing state and morphological mixing state, and the deliverables that address each aspect. See Section 5.1 for descriptions of deliverables D1-D13. Despite the fact that many tools by themselves have a high readiness level, the output of these tools is typically not directly comparable (see Table 2). The difficulties in comparison is a primary bottleneck in understanding mixing state. The entries under "readiness level" are color-coded according to high level of readiness (green), medium level or readiness (yellow), and low level of readiness (red). The entries under "deliverables" are color-coded according their status of funding (funded, proposed, planned).

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GCM	low	D3, D4, D13	low	
SP2	medium	D5, D6, D8, D10, D12	medium	D6, D10
Microscopy	medium	D1, D8, D12	high	D6, D5
Single-pa spetromet				

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We don't deal well with modeling morphology.
How can we improve this?

Table 4:
Integration of Field Campaigns and Modeling

Campaign	Measurements	Models		
		PRM	RM	GCM
MILAGRO	D1			
CARES	D1, D5, D8	D8	D4	D3
ClearfLo	D5			
TCAP	D8	D8	D4	
GVAX	D7		D7	
BBOP	D14			
Laboratory	D6, D9	D6, D9		

Table 4: Integration of deliverables with observational data from recent field campaigns and modeling work. The colors indicate coverage level (green: well-covered; yellow: some coverage; red: no coverage).

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Laboratory	D6, D9	D6, D9		

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We don't have a model hierarchy in place.
How can we improve this?

Overview of Deliverables

funded

D1: Mixing state metrics from microscopy

Moffet, Gilles, Laskin, Sellon

D2: PartMC-3D and error quantification

West, Riemer

D3: Error bounds for mixing state modeling in GCM

McGraw

D4: Development of MOSAIC-mix

Zaveri, Easter, Fast

D5: Characterize single-particle morphology in different environments

Subramanian, Mazzoleni

D6: Chamber experiments and PR modeling of Soot Aging

Shilling, Zaveri, Zelenyuk, Sedlacek,

D7: Biomass burning mixing state analysis during GVAX with WRF-Chem

Feng, Kotamarthi

proposed

D8: Validating PR model simulations with observations from CARES and TCAP

Riemer, Fast, Zaveri, West

D9: Improve models of surface tension to improve representation of morphology

Anthony Wexler, Simon Clegg, Cari Dutcher

D10: Chamber experiments and PR modeling to study mixing state

Davidovits, Lambe, Lewis, Onasch, Sedlacek

D11: Including morphology information in PartMC-3D for improved radiative forcing estimates

Scarnato, Mazzoleni, Riemer

planned

D12: Single-particle instrument intercomparison

TBD

D13: Mixing state modeling obstacle course

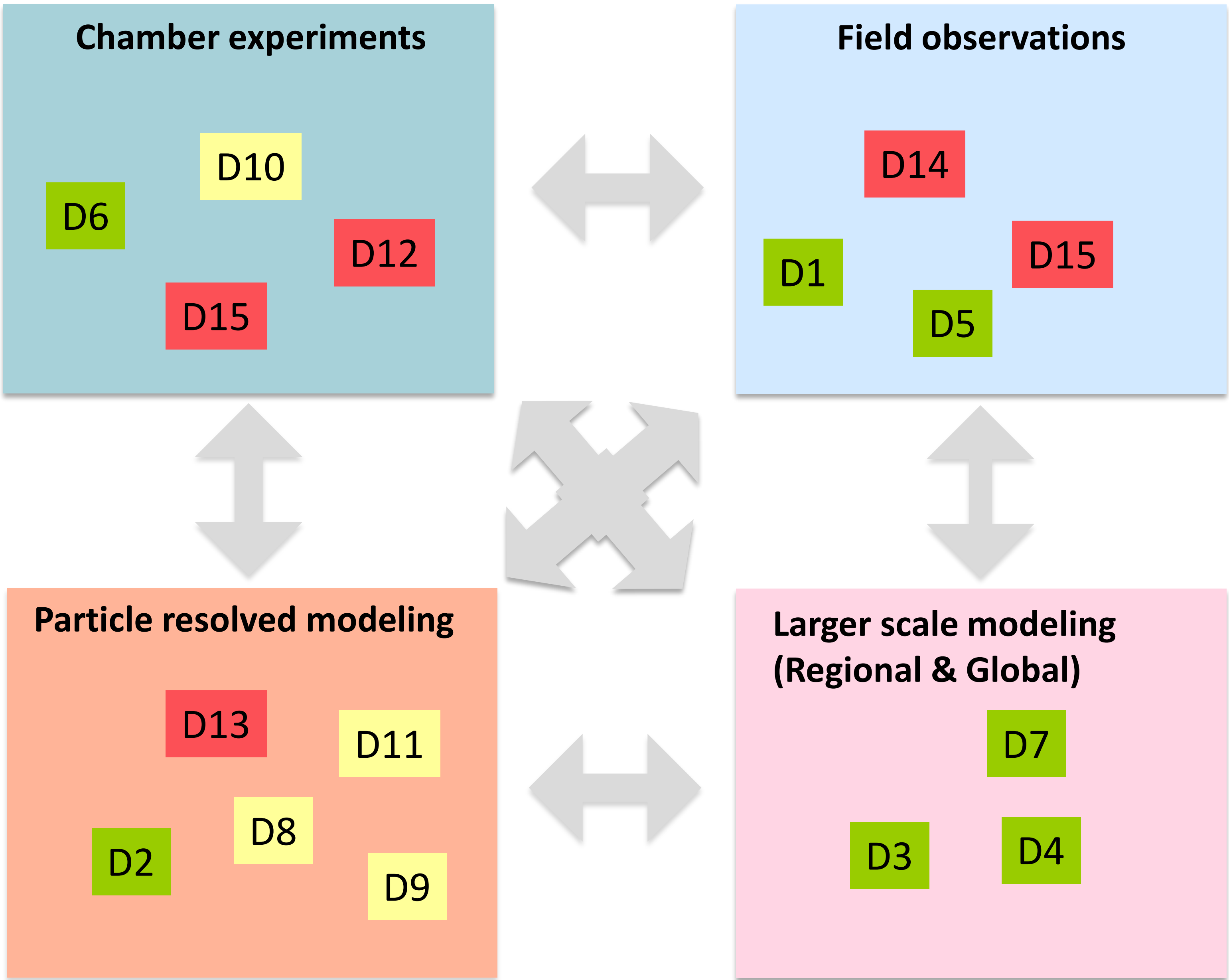
Riemer, West

D14: Mixing state analysis and modeling during BBOP

Adachi, Buseck, Onasch, Sedlacek

D15: BC/BrC Mixing state as a function of age: Laboratory (FLAME, BC) to Field (Clearflo, CARES, BBOP?) for Model

Dubey, Mazzoleni, Cappa, Aiken, Donahue, Zaveri, Fast, Feng


Chamber experiments
D10
D6
D12
D15
Field observations
D14
D1
D15
D5
Particle resolved modeling
D13
D11
D8
D2
D9
Larger scale modeling
(Regional & Global)
D7
D3
D4