

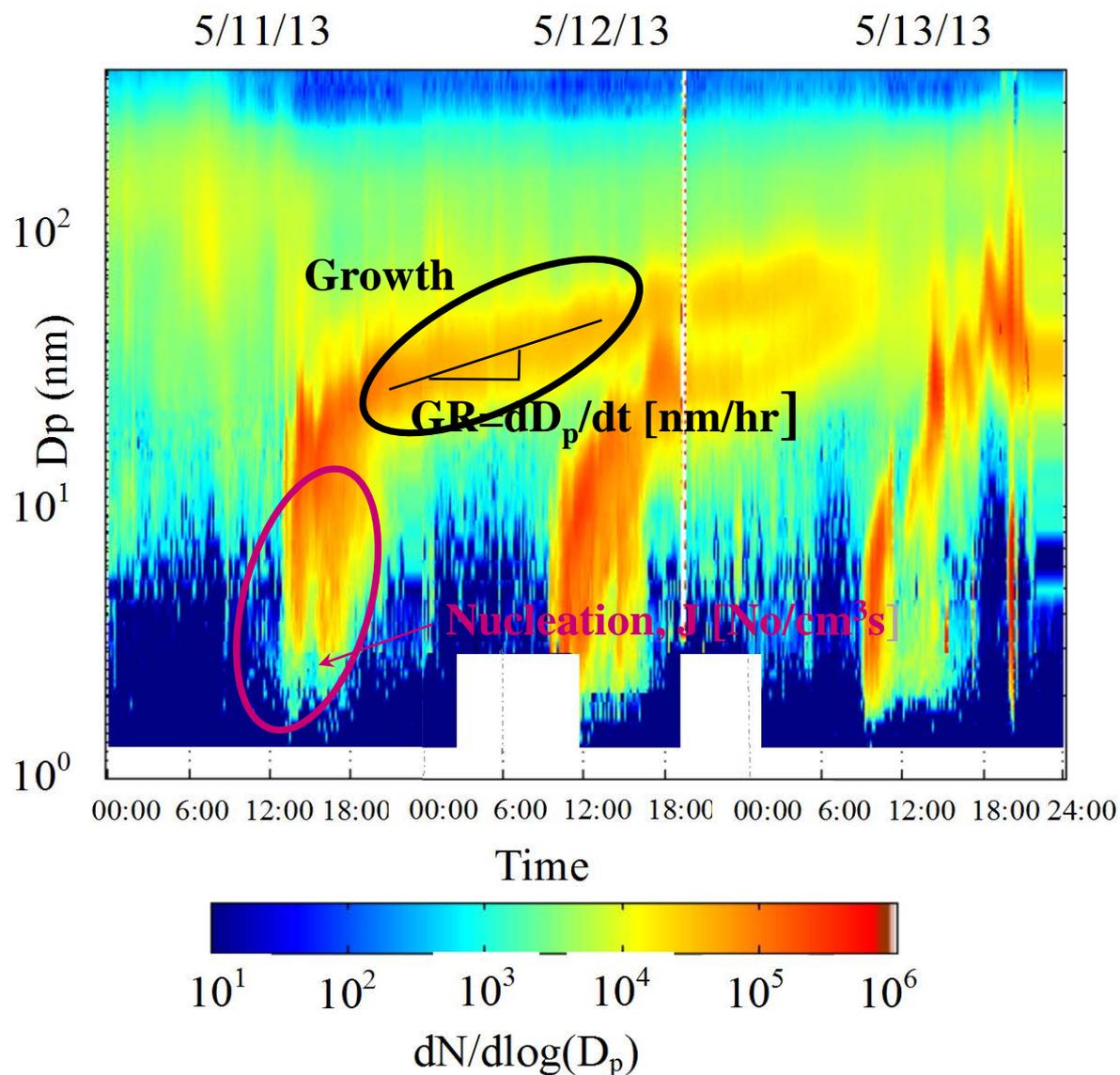
# **New Particle Formation (NPF) Focus Group**

**Chongai Kuang, BNL**

**Peter H. McMurry, U Minnesota**

**James N. Smith, NCAR**

# New Particle Formation (NPF) Events, May 11-13, 2013. Lamont, Oklahoma, US



# Focus Group Objectives

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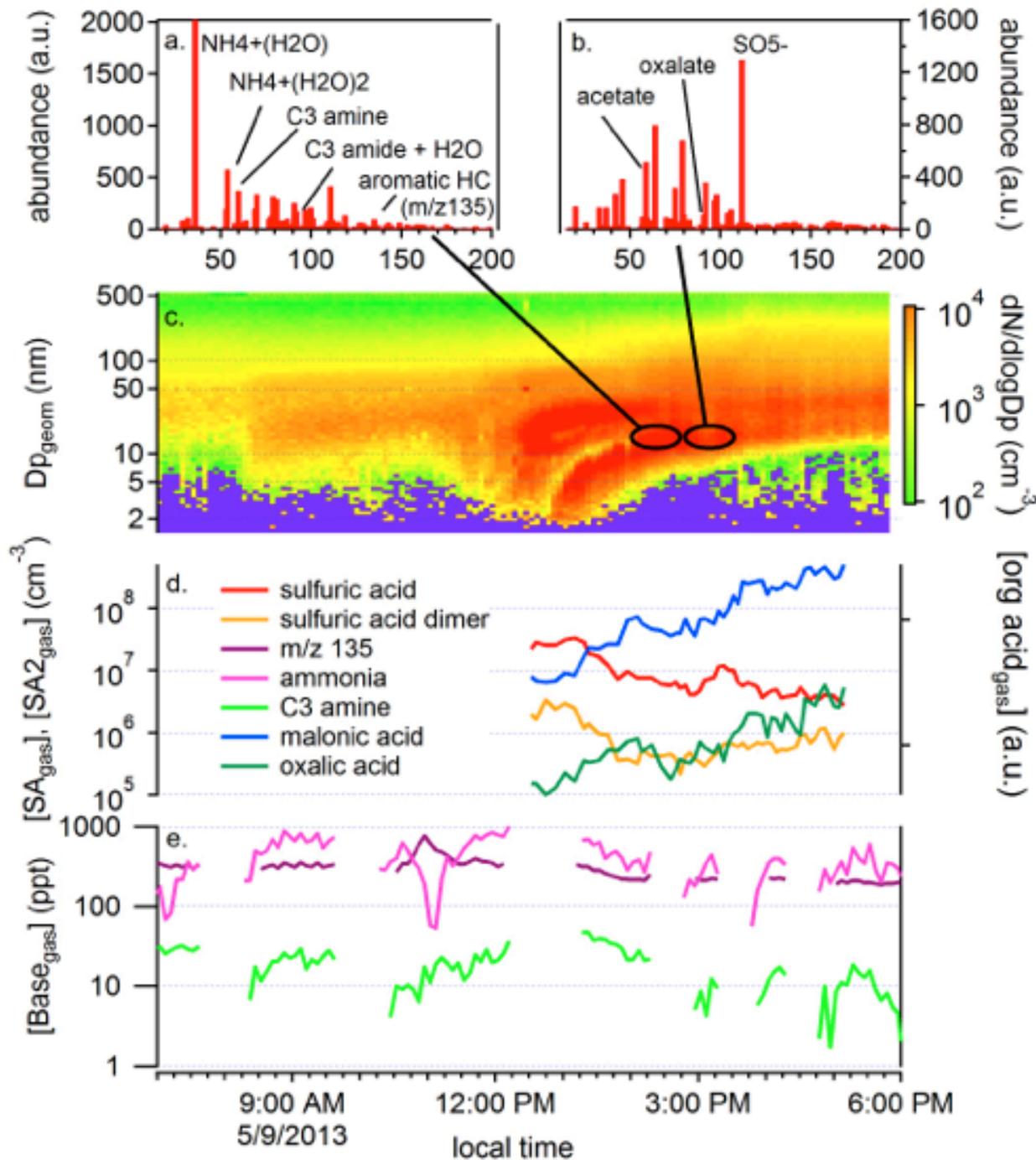
- 1. Develop empirical and first-principles models for
  - *nucleation rates*
  - *growth rates*
  
- 2. Use observations to determine climatically important physico-chemical properties of the aerosol formed by nucleation such as hygroscopicity, phase, and surface tension.
  
- 3. Incorporate NPF models into regional models.
  
- 4. Incorporate NPF models into global climate models.

# Approach towards Achieving Objectives

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- 1. IMPROVED INSTRUMENTATION:
  - Gas phase precursors
  - Particle composition
  
- 2. Atmospheric Observations
  
- 3. Theoretical Model Development Coupled to Laboratory Research
  
- 4. Validation and Application of Atmospheric Models

# Parallel Measurements of Precursor Vapor and Particle Composition During a Nucleation Event at DOE's Southern Great Plains Site on May 9, 2013



# Key Scientific Challenge: Understanding Mechanisms by which Organic Compounds Contribute to Growth

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Organics typically account for 90% of growth

$$\triangleright GR = (5-10) * GR_{H_2SO_4} = GR_{H_2SO_4} + GR_{other}$$

Diverse reaction pathways likely contribute to organic uptake

$$\triangleright GR_{other} = GR_{acid-base} + GR_{accret} + GR_{rev\ cond}$$

# Focus Group Participants

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- NCAR, CSU, UMN, Augsburg, Portland State team
  - Jim Smith, Jeff Pierce, Pete McMurry, Dave Hanson, Kelley Barsanti
- BNL
  - Chongai Kuang, Jian Wang
- Others
  - SOA uptake; Computational chemistry, etc.
- International: U Helsinki (Kulmala, Worsnop)
- Other modeling groups

# A Vision for Optimizing Effectiveness of NPF Focus Group

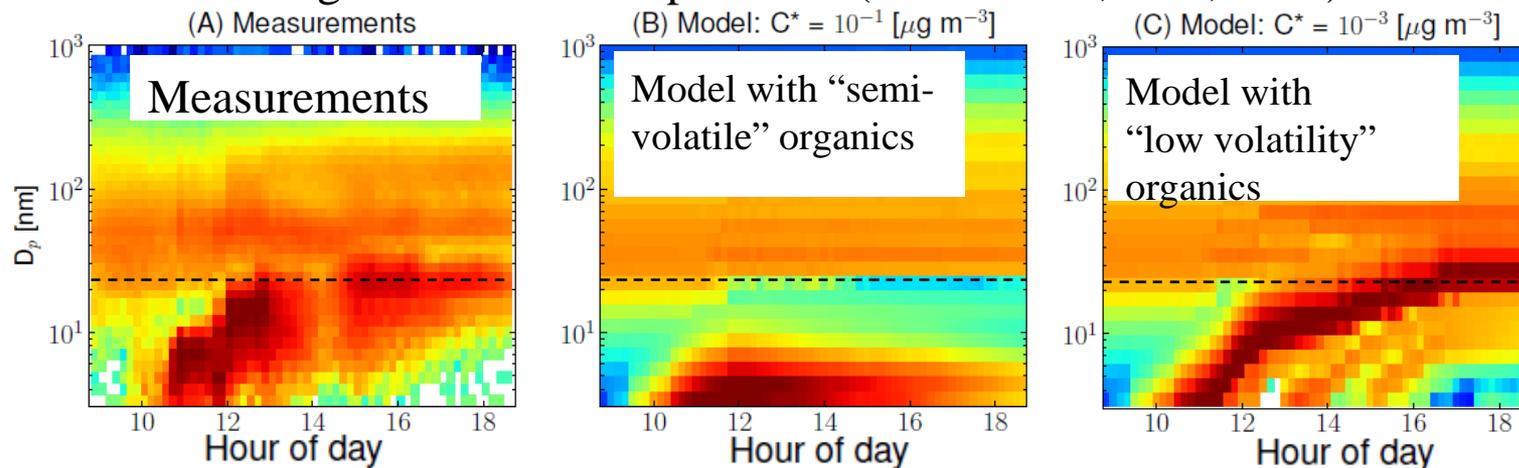
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- Tightly knit, collaborative team
- Complementary objectives
- Flexibility
- Periodic (annual?) meetings that focus exclusively on NPF

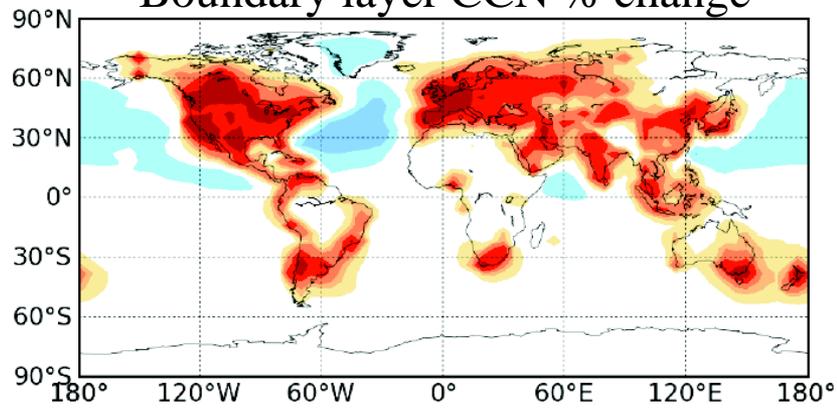
# **Some Recent Activities**

# NPF and Growth in Models (Jeff Pierce)

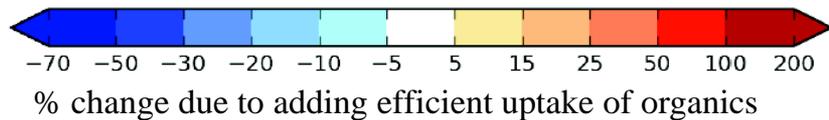
Models cannot capture the growth of new particles without efficient uptake of organics to the new particles. (Pierce et al., ACP, 2011)



## Boundary layer CCN % change



CCN concentrations in the continental boundary layer are very sensitive to this efficient uptake of organics to new particles. (D'Andrea et al., ACP, 2013).



### Inputs / Observations

- $[H_2SO_4]$
- BVOC oxidation rate
- $[NO_x]$
- $[NH_3]$  & [amines]<sup>a</sup>
- $A_{Fuchs}$
- Size-dependent aerosol acidity
- T, RH

Photochemical model<sup>b</sup>

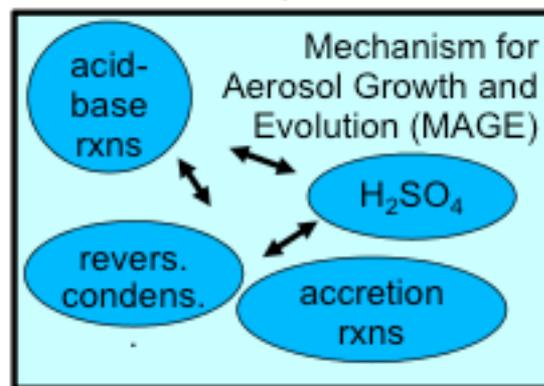
### Precursors

- -dicarbonyls
- semivolatile vapors

Aerosol Growth Rate Estimator (AGRE)

### Outputs

- $GR(D_p)_{H_2SO_4}$
- $GR(D_p)_{BVOCox}$
- $GR(D_p)_{NH_3}$
- $GR(D_p)_{amines}$



### Outputs

- $GR(D_p)_{H_2SO_4}$
- $GR(D_p)_{acid-base}$
- $GR(D_p)_{accret}$
- $GR(D_p)_{rev cond}$

#### Notes:

<sup>a</sup>In cases where amine observations are not available,  $NH_3$  concentrations will be used to develop estimates.

<sup>b</sup>Box models such as GECKOA could be used to estimate precursors where observations are missing.

## Approaches to Modeling Growth:

Mechanistic (MAGE)

and

Empirical (AGRE)

# Discussion...