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

\[ \text{Growth} \]
\[ \text{GR} = \frac{dD_p}{dt} \text{ [nm/hr]} \]

\[ \text{Nucleation} \]
\[ J \text{ [No/cm}^3\text{s]} \]
Focus Group Objectives

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

□ 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

Organics typically account for 90% of growth

\[ GR = (5-10) \times GR_{H_2SO_4} = GR_{H_2SO_4} + GR_{other} \]

Diverse reaction pathways likely contribute to organic uptake

\[ GR_{other} = GR_{acid-base} + GR_{accret} + GR_{rev cond} \]
Focus Group Participants

- 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

- 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)

Measurements

Model with “semi-volatile” organics

Model with “low volatility” organics

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).
Approaches to Modeling Growth:

Mechanistic (MAGE) and Empirical (AGRE)

Notes:
- In cases where amine observations are not available, NH₃ concentrations will be used to develop estimates.
- Box models such as GECKOA could be used to estimate precursors where observations are missing.
Discussion...