White Paper

New Particle Formation Focus Group

Preface

Atmospheric chemical transformations can lead to New Particle Formation (NPF). NPF is a two-step process. First, nucleation leads to the formation of tiny stable nuclei, which are probably about 1 nm in size. A stable nucleus is one that is more likely to grow than to evaporate. Then, to have an effect those nuclei must grow to a larger size. The NPF effect of greatest concern in climate research is on concentrations of cloud condensation nuclei (CCN). Particles must grow to sizes of about 50 nm or larger before they are large enough to serve as CCN. In addition to particle size, chemical composition and surface properties also play an important role in determining the likelihood that a particle can activate into a cloud droplet. Nucleation rates determine how many newly-formed particles could potentially serve as CCN. Growth rates determine whether or not nucleated particles will actually reach CCN sizes before they are lost by coagulation with pre-existing particles. The chemical species that contribute to growth determine the composition of the potential CCN. Previous research has shown that both nucleation and growth rates are much higher than were predicted by early naïve models. The goal of this focus group is to develop models that accurately predict nucleation and growth rates and the composition of potential CCN, and to incorporate these into regional and global atmospheric models.

Objectives

1. Develop models for *nucleation rates* and *growth rates* of atmospheric nanoparticles.

-develop empirical models that accurately describe atmospheric observations (a short term objective that would be of value).

-develop first-principles models for the dependence of these rates on concentrations of participating gas phase species (a primary goal of this research).

-Use observations of the chemical species and mechanisms responsible for growth to determine climatically important physico-chemical properties of the aerosol formed by nucleation such as hygroscopicity, phase, and surface tension.

2. Incorporate mechanistic models for nucleation and growth rates into regional models to assess model performance during intensive atmospheric observations in well-defined environments.

3. Incorporate these models into global climate models to quantify the effects of new particle formation on climate.

Approaches

Model Development: The development of experimentally verified models for nucleation and growth rates in the atmosphere will require a multidimensional approach.

1. Instrumentation. Measurements of (i) gas phase species that participate in nucleation and growth and of (ii) the composition of clusters and nucleated particles formed are required. Such measurements will allow proposed mechanisms to be tested experimentally. Instruments that can carry out such measurements have advanced rapidly over the past decade, and more instrument development will be required.

2. Atmospheric Observations. Models do not yet predict which species participate in atmospheric nucleation and growth. Therefore, atmospheric observations are needed to empirically identify those species, and where possible, to define the functional dependencies of nucleation and growth rates on their concentrations. These measurements should include vertical gradients and seasonal variability of the physico-chemical properties of freshly nucleated aerosols. Vertical gradients are required since a crucial part of understanding the impacts of new particle formation on climate is understanding the transport of trace gases and aerosols into regions of the atmosphere where supersaturations are high enough to activate these aerosol into clouds (i.e., at cloud base). Information on seasonal variability is required because new particle formation has been observed year-round in most locales. The required observations can leverage existing DOE activities such as the remote sensing and long-term observations at the ARM SGP site and field campaigns. Using NPF measurements from such long term observations, valued added products (VAPs) can be developed that concisely characterize the survival of freshly nucleated particles as they grow to climate-relevant sizes. These NPF VAPs will provide needed observational inputs and constraints to the aerosol micro-physical/chemical modules contained in regional and global climate models.

3. Laboratory Studies. Laboratory studies under well-controlled conditions are needed to develop accurate mechanistic models for nucleation and growth rates, and to determine climatically important aerosol properties. The laboratory studies will quantify the dependence of rates and composition on variables that include temperature and concentrations of the reacting species, including water vapor.

Model Validation: The micro-physical/chemical models for nucleation and growth will be incorporated into regional models and compared with intensive atmospheric measurements. This work will allow a comparison of direct measurements and of regional model predictions for both the concentrations of the precursor gases that contribute to nucleation and growth, and nucleation and growth rates.

Global Modeling: Models for boundary layer nucleation and growth rates that have been verified in atmospheric studies will be incorporated in global climate models such as CAM5, in collaboration with Xiaohong Liu at PNNL.

Leadership

Peter McMurry (University of Minnesota), James Smith (National Center for Atmospheric Research) and Chongai Kuang (Brookhaven National Laboratory)are willing to lead this Focus Group.

Metrics for Evaluating Progress

1. Publication of papers that describe advances in measurement methods for the concentrations of gas phase precursors and the composition and size distributions of freshly nucleated particles.

2. Publication of experimentally-verified model(s) for nucleation rates.

3. Publication of experimentally-verified model(s) for growth rates.

4. Publication of comparisons between predictions of regional models and atmospheric measurements.

5. Publication of papers that describe the effect of new particle formation on climate.