A White Paper on

Climate, Atmospheric Processes and Air Quality: Providing Fundamental Insights and Tools for the Next Advances Through the Mathematical and Physical Sciences[1]

MPSAC Members: Taft Armandroff, James Berger, Paul Butler, Barbara J. Finlayson-Pitts, Iain Johnstone, Michael Norman, Elsa Reichmanis and Fred Roberts
NSF Staff Members: Tom Carruthers and Zeev Rosenzweig

[1] We gratefully acknowledge comments and suggestions from Bill Cooper, Nina Fefferman, Chris Jones, Sam Shen and Richard Smith.

May 18, 2011

Executive Summary:

Climate change and its impacts clearly represent one of the greatest challenges facing civilization today. Models that integrate existing knowledge of the processes and species that affect climate play a critical role in elucidating the complex interrelationships involved in past climate changes, the impacts of anthropogenic and biogenic emissions, and the likely impact of changes in future emissions. Key to these models is accurate input data and analytical techniques, much of which comes from the Mathematical and Physical Sciences community. Some examples where MPS can, and should, make a significant contribution include:

- Development of fundamental, molecular level understanding of the key chemical and physical processes involved in climate change, particularly those involving the formation and fate of airborne particles;
- Development of new computational and visualization tools to handle the massive amounts of relevant data;
- Development of new techniques for the quantification and presentation of model uncertainties and sensitivities;
- Development of new tools to integrate across the vast geographical and temporal scales involved in climate change;
- Development of new tools to integrate across disciplines such as the mathematical/ physical sciences and the economic/social/behavioral sciences in order to reliably predict feedbacks between them.

MPS is uniquely situated to provide such fundamental data, and in addition, to form partnerships across disciplines that will be key to addressing climate change and its impacts.

Background

Climate change is clearly one of the greatest challenges faced by civilization today. Fundamental understanding of atmospheric processes and coupling between the atmosphere, oceans and biosphere is critical for providing policy makers with accurate information needed to develop cost-effective strategies for monitoring, control, mitigation and adaptation. Many published studies have documented the current state of understanding of climate change and the key challenges and uncertainties that remain; see for example, those from the Intergovernmental Panel on Climate Change[4] and the National Academy of Sciences (a list of available documents is found at http://dels.nas.edu).

Figure 1 summarizes the calculated changes in radiative forcing since the year 1750. Radiative forcing is the change in the average net radiation at the tropopause due to a perturbation that alters incoming or outgoing radiation. Because it is directly related to the associated temperature change at the Earth's surface, it is used as a proxy for assessing the contributions of various species or perturbations to climate change. A positive value of the radiative forcing leads to warming and a negative value to cooling.

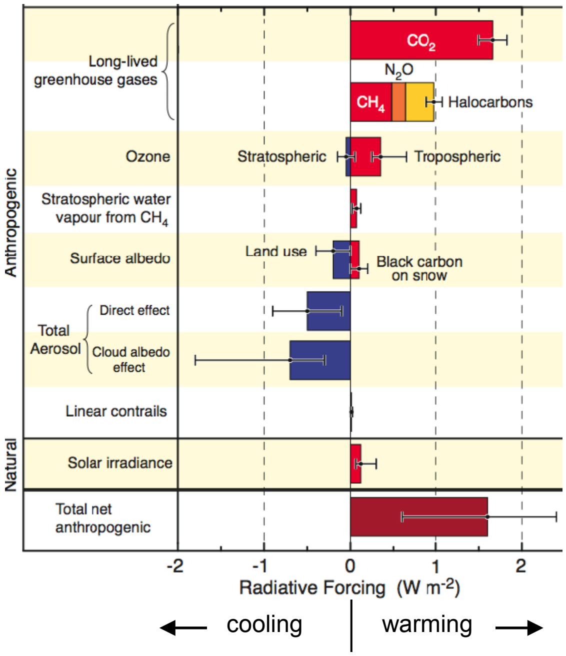


Figure 1. Estimated contributions to changes in radiative forcing since 1750 (Intergovernmental Panel on Climate Change, 2007)

The data in Fig. 1 show that changes since the industrial revolution in CO_2 as well as methane, nitrous oxide and the halocarbons contribute to positive radiative forcing. Tropospheric ozone, an air pollutant for which air quality standards are set, also contributes ~20% of that due to CO_2. These, along with water vapor, comprise the well-known greenhouse gases.

However, there are some perturbations, in particular an increase in airborne particles, that are believed to have partially counterbalanced the warming associated with the greenhouse gases. Furthermore, it is clear that the largest uncertainties (shown by the bars in Fig. 1) in the final net radiative forcing due to anthropogenic activities arise from airborne particles. Particles directly cause negative radiative forcing, i.e., cooling, due to direct light scattering, while absorption of light by soot and other components gives a positive radiative forcing, i.e., warming.[4-7] Particles also have an indirect effect on climate via changing cloud properties such as the number concentration and size distribution of cloud droplets, which changes their light scattering (albedo), their lifetimes and precipitation rates.[8-20] Changing particle concentrations may be responsible for the rapid climate change that is not well captured by current climate models.[21-23]

In addition to their impacts on climate, airborne particles have been associated with cardiovascular disease, lung cancer and asthma,[24-27] and have also been directly linked to increased mortality for almost a century.[28,29] Because species that have traditionally been considered as air pollutants (e.g., ozone, particles) also play central roles in climate change, it is critical to consider atmospheric processes, air quality, atmospheric processes and climate change as facets of the same phenomenon, rather than as separate issues.

Challenges

Models are used to integrate existing knowledge of the processes and species that affect climate. Such models play a critical role in elucidating the complex interrelationships involved in past climate changes, the impacts of anthropogenic and biogenic emissions, and the likely impact of changes in future emissions. Models are run on different geographical scales, from local to regional and global, and a broad range of temporal scales, from minutes to decades or longer. As the magnitude of the scales increase, so does the model complexity. The broad scales of distance and time that must be encompassed by global climate models are such that including, for example, comprehensive, molecular level chemistry is not currently feasible. Similarly, there are challenges in how to mathematically represent important sub-grid-scale phenomena such as cloud formation and evaporation in a manner that accurately represents the underlying processes. Thus, simplified parameterizations of a number of key processes must be developed for inclusion in climate models. A key requirement for such parameterizations is ***understanding the underlying fundamental science.*** Only with such insight can the necessary larger scale parameterizations be developed and integrated into predictive models with confidence. Furthermore, ***integration of new knowledge and its presentation in forms useful for different audiences***, which is critical for providing guidance to the scientific community, the public and policy makers, requires the development of new approaches in ***data mining and data analysis as well as visualization techniques and new decision support tools***.

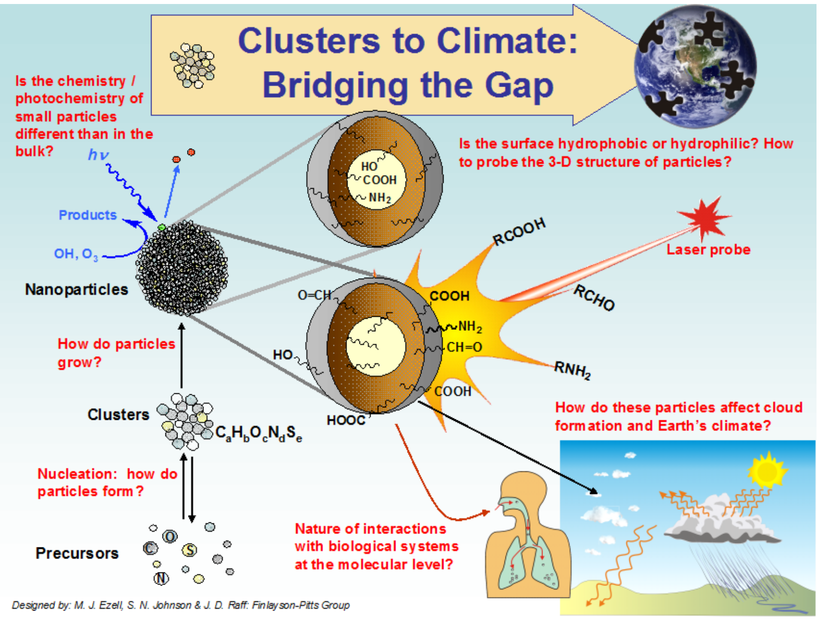
The scales and complexities of issues involved in climate change are such that knowledge across many disciplines must be integrated. This includes not only geosciences and engineering, but also the mathematical, physical and biological sciences, computer sciences and the social, behavioral and economic sciences.

Role of the Directorate for Mathematical and Physical Sciences (MPS)

Mathematical and Physical Sciences at NSF has key roles to play *in providing the fundamental scientific data and tools needed to advance our understanding of the physical basis of climate change, developing mitigation and adaptation strategies based on sound science, and in providing the tools to incorporate this fundamental knowledge into models that are useful to a variety of audiences.* The latter include researchers focusing on various aspects of climate change, atmospheric processes and air quality as well as policy makers, legislators, regulators and the public. Of course, efforts within MPS must be hand-in-glove with other directorates at NSF that bring different expertise and perspectives to the table.

Some examples of the areas in which particular expertise found within MPS can contribute to advancing climate science follow.

A. Understanding the Fundamental Chemical and Physical Processes.



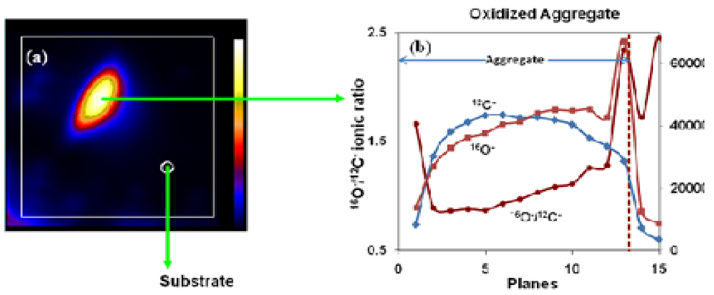
Designed by: M. J. Ezell, S. N. Johnson & J. D. Raff: Finlayson-Pitts Group

Figure 2. Depiction of some key problems connecting particles to climate and air quality.[1]

As seen in Fig. 1, particles play key roles in climate change, and furthermore, it is their impact on climate that introduces the greatest uncertainties into simulations of the past, and model predictions of the future climate. In addition, most geo-engineering schemes proposed for mitigation rely on introducing particles into the atmosphere. There are a myriad of unsolved, fundamental problems concerning the formation, growth and fates of airborne particles to which MPS can contribute. Some key questions that remain to be answered are depicted in Fig. 2 and summarized below.

- What are the nucleation processes that first form clusters and subsequently result in the growth of new particles in air? What species are involved? What is the role of water? How do particles grow? Once a particle nucleus is formed, what determines the uptake of gases onto and into the particles that causes them to grow? The driver for this is that a major role of particles in climate change is their ability to take up water and act as cloud condensation nuclei, CCN (or ice nuclei, IN). There is clear evidence from field studies that the presence of particles that can act as CCN results in a greater number of smaller cloud droplets for a given liquid water content. If the drops are not sufficiently large to rain out, precipitation rates are affected. In addition, cloud lifetime and albedo (light scattering) are increased, enhancing the impact of particles on climate.

- How do the properties of clusters and new nanoparticles compare to those of the corresponding bulk phases? What molecular level interactions contribute to differences between the clusters and bulk phases? For a particle with a 1.0 µm diameter and typical atmospheric composition, only ~1% of the molecules are on the surface; at 50 nm ~25% are surface molecules; but at 3 nm, 100% of the molecules on the particle can be considered to be surface species! The chemical, photochemical and physical properties will clearly change across this range of sizes of atmospheric clusters and particles, but how and why is not well understood.
- What is the 3-D structure of particles, including identification of the specific organic components? What processes lead to these 3-D structures? It has been the traditional expectation that particles formed in organic oxidations in air will be quite polar and readily take up water. In one laboratory study, however, nano-SIMS of particles formed by oxidation of an organic monolayer on a surface showed that the polar groups were actually buried inside the particles (Fig. 3).[3] Research in the field of materials science, for example, on self-assembly, may shed some light on this area. Particle composition has been measured historically by collecting particles on filters and carrying out bulk chemical analysis on the extracts. Over the last decade or so, some elegant particle mass spectrometry techniques have come online. However, none of these yet provide



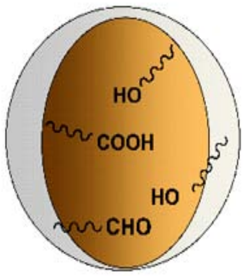


Figure 3. Nano-SIMS analysis of particles from ozonolysis of an alkene self-assembled monolayer showing polar groups buried inside particle and cartoon of possible 3-D structure.[3]

speciation of organics, or the capability of 3-D profiling, i.e., peeling them apart like an onion. In addition, the functional groups on the surface need to be identified and measured. *3-D* imaging with *chemical speciation* on *single particles* in *real time* down to ~ *1 nm* in size is the ultimate goal. This will require new analytical approaches that will also have a number of other applications, for example to biological systems.

- What is the chemistry and photochemistry that occurs in and on particles? This chemistry leads to changes in their composition and also determines their light scattering and absorption as well as lifetimes in the atmosphere. Is the chemistry and photochemistry different at the surface compared to the bulk?

B. Development of New Computational and Visualization Tools.

Since we have only one Earth we need mathematical replicas, in the form of Global Climate or Earth System Models, to give us a laboratory for both scientific hypothesis testing and projections of future states of the planet. At the same time, there are dramatically increasing amounts of observational climate data. Figure 4 shows the amounts of climate data from model outputs, remote sensing observations and *in situ* measurements estimated to be generated over the next two decades.[2] Extracting the highest value from such data sets, and the use of that information in both model improvement and design of new observational strategies, will require new computational as well as data visualization tools.[30]

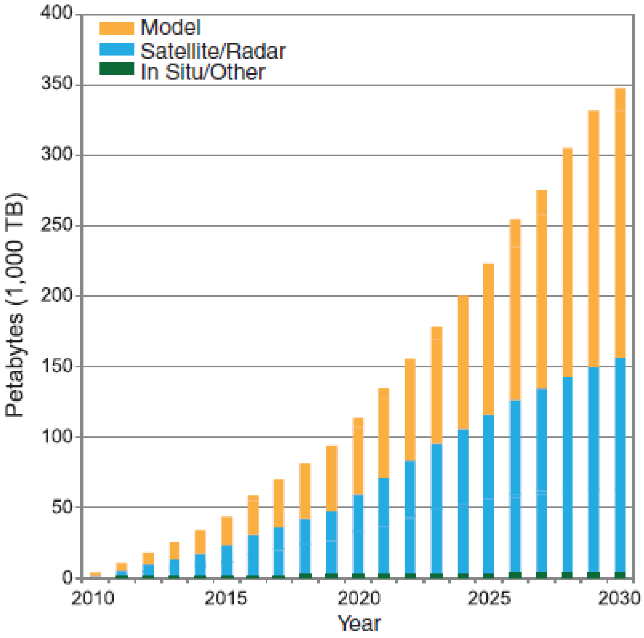


Figure 4. Estimated climate related data generation for next two decades. From Overpeck et al.[2]

Some examples are summarized in the following. Others under this and the following sections are included in a report on mathematical challenges for sustainability that is forthcoming from a workshop on that topic sponsored by six North American mathematical sciences research institutes in November, 2010. It will be added as an appendix to subsequent versions of this white paper.

- Increasing computational power allows us to model processes that were only parameterized in earlier models. But this can introduce new instabilities and uncertainties and thus poses challenges at all levels of computational modeling, including the need for novel numerical codes such as self-adjusting schemes that can intelligently adapt their resolution.
- The extraordinary advances in computer modeling also call into question the strategy of incrementally building climate models within the mold of their predecessors. We will make the largest strides by rebuilding climate models from scratch. The current complexity of Earth System Models makes this a daunting, but very exciting, challenge.
- Observational data and models are both used intensively in climate research. They have not been used in concert to anything like the same extent as in Numerical Weather Prediction. There are enormous benefits to be reaped from a systematic approach to assimilating data into climate models. This would lead to steps forward in: model calibration and tuning, model parameter identification, model validation and verification, uncertainty quantification as well as the identification and elucidation of scenarios that are not well understood. In addition, abrupt and extreme events are generally not captured by models and are not well understood; the development of new tools using assimilation of available data may help considerably in this regard.
- Physical modeling of complex and nonlinear systems such as quantum dynamics, chaotic systems, turbulent transport, and the statistical dynamics and thermodynamics of large systems have resulted in computational techniques that should be adaptable for climate studies. Collaborations between the developers of these modeling systems and experts in climate studies may provide new accurate and robust modeling techniques. Similarly, adaptation of the tools of statistical physics, as opposed to brute-force numerical modeling simulations, may simplify and increase the accuracy of climate models.
- Also needed are new statistical tools and machine learning and data mining techniques that will provide the most rapid alerts to anomalies resulting from climate change, for example, in biodiversity, extreme events such as large hurricanes, water shortages and changes in physical, chemical and oceanographic data such as ocean pH.
- Development of new methods is needed for presenting data, for example visualization of massive data sets, that can help us gain better understanding of the state of natural systems and of changes in them.

C. Quantification and Presentation of Uncertainty and Sensitivities.

Uncertainty is inevitable with models of complex systems such as climate, both from individual models and from the differing conclusions arising from different models. Climate models have numerous individual inputs, each with its own uncertainties, that combine in ways that are often non-linear, non-stationary and inhomogeneous, and with sometimes surprising or unexpected results. In addition, model predictions are more sensitive to some inputs than others; those to which the model outputs are most sensitive may also depend on the particular output parameter of interest. Understanding model sensitivity in a quantitative fashion provides guidance on which input parameters might first be studied in order to have the greatest in impact on reducing model uncertainties. When different models lead to different conclusions, techniques are needed to reconcile the differences or find “averaging procedures” that take account of differing assumptions and varying quality of data.

In short, quantitative treatments of both model sensitivity and uncertainty are critical to the scientific community, policy makers, regulators and the general public. Some needs in this area to which MPS could contribute include the following:

- The optimal assimilation of available climate data with sensitivity and uncertainty estimates will be critical to the objective and conclusive assessment of climate change and its impacts. New tools are needed to develop high quality observational datasets and estimate their errors, as well as to quantify the sensitivities of the data to relevant parameters. In addition, techniques to extract the extent to which an observed climate change can be attributed to different forcings are needed.
- The particular input/output data of interest may vary depending on the question being asked. Understanding and quantifying such sensitivities is critical for identifying important areas for further study as well as the optimal use of resources and efforts by various communities. For example, at the heart of conservation biology, which is intimately related to climate change, is the problem of the optimal allocation under rigid economic and sociological constraints of scarce parcels of land, wetland, and marine environments needed to preserve extant biological communities and to provide areas for the restoration of ecosystems and reintroduction of locally extinct species. Tools for evaluating the sensitivity of models of optimal allocation to changes in climate that might affect availability and “quality” of habitat would be very useful.
- Further development of tools is needed to express and quantify model uncertainties, either from an individual model or from an ensemble of models, in ways that are meaningful to various audiences. This includes not only the treatment of temperature, but also other variables such as precipitation and hurricane intensity and frequency, for which the statistical and mathematical techniques needed may differ substantially.

D. Development of Tools to Integrate Across Geographical and Temporal Scales.

Geographical scales of interest vary from local to regional to global, with temporal scales from a few hours to decades or more. The development of a variety of new tools to integrate across scales is essential for understanding the subtleties of climate change. For example:

- The impacts of climate change and atmospheric processes are experienced on a local scale, yet tools for predicting local and regional scale effects from global scale phenomena are not well-developed. Conversely, what begins as a local or regional scale effect or emission on short time scales becomes in aggregate a global scale effect on longer time scales. Reliable tools for coupling these ranges are critical for understanding the impacts of climate change and developing optimal adaptation and mitigation strategies. In most cases, there will be multiple optimization criteria. Although multi-criteria decision making is a well-developed field within operations research and related areas of economics, levels of uncertainty are often much higher in the case of climate change than are standard within operations research and economic modeling, and new algorithms are needed that utilize stochastic optimization in such cases. Similarly, questions such as the following need to be addressed: When is a dynamic downscaling (such as using a regional climate model to interpolate within the grid cells of a global climate model) superior to statistical downscaling (i.e., developing direct relationships between the variables of the global model and the local variables of interest)?
- Challenges of modeling sustainable biodiversity are also multiscale (including migration, meta-population dynamics, species diffusion and invasion, food webs, etc.) and these scales cross many different environments, each likely to be affected by the same climate change in drastically different ways. Tools that will integrate local models of the impact of climate change to produce global perspectives (especially across land-sea-air ecosystem boundaries) are needed.
- The development of a systematic approach to the reduction of model complexity, so as to build a hierarchy of climate models, amenable to varying degrees of mathematical analysis and interpretation is needed. Transfer of information among the hierarchy of models is important but it is not realistic to rely on rigorous reductions. Conceptual models can reveal effects that will be hidden in big models, but there is no common agreement as to how to use information from simple models to inform big models.
- Tools to optimize the design of monitoring and measurement systems, and to optimize data analysis from such networks to provide the parameters of interest, are needed.

E. Development of Tools to Integrate Across Disciplines.

The issue of climate change covers a broad range of impacts (e.g., economic, social, ecological) and feedbacks (e.g., behavioral). As stated in a recent National Academy of Sciences report:[31]

> *Addressing these issues requires the integration of disciplinary and multidisciplinary research, natural and social science, and basic research and practical applications.*

This has been described as a "new paradigm that joins traditional climate research with research on climate adaptation, services, assessment and application". [2]

Climate change research requires fundamental new methods that integrate tools of the mathematical and physical sciences with tools of other disciplines. For example:

- Climate change is critically related to the interplay between natural and human systems. The development of tools to integrate physical models of climate, atmospheric processes and air quality with socio-economic, behavioral and risk models is urgently needed in order to couple predictions of climate change with its impacts and behavioral changes that can aid in, or hinder, adaptation and mitigation. This calls for a new stress on integration between the mathematical, physical and social sciences. For example, what tools can be used to assess the impact of one meter sea level rise on island nations, and as these nations disappear, to evaluate and assess those losses? Can the social disruptions and conflicts be modeled in order to predict and mitigate effects such as shortages or surpluses in the availability of food, water, etc.? Can models of mathematical epidemiology be modified to understand the effect of climate change on diseases of people, animals, and plants, and to incorporate our understanding of these changes into control strategies? Can tools be developed to assist in adapting to climate change, for example, the development of algorithms for locating evacuation facilities, assigning evacuees to facilities, and choosing transportation routes that will minimize cost/disruption/impact of evacuations?
- Can economic models be developed that incorporate concepts of sustainable economic development but also be connected to physical models of climate and environmental quality? Can models be developed that lead to fundamental understanding of how different alternative combinations of energy sources, energy production, energy storage, energy distribution, and energy use protocols affect climate as well as how they interconnect with economic processes?
- Natural resources (water, wood, fish, etc.) are fundamental to a sustainable lifestyle. How can the effects on water supplies of changing agricultural practices due to climate change be modeled, and how can these models be used to predict regional water shortages from a changing climate? How can the future health of fish populations be predicted when their normal healthy environment is affected by changing temperature/humidity/seasons? What policies for allocation of scarce resources are most “equitable” in a precise mathematical sense?
- Climate change models have predicted a decreased stability in environmental/ meteorological characteristics of habitats and the increased fluctuation may have climate-specific patterns that connect to the health of populations in an ecosystem that need to be studied. For example, mathematical analysis of stochastic fluctuations in small populations due to climate, though well studied, faces significant challenges due to increased environmental instability. Similarly, how can changing climatic conditions and resulting diseases of different species be included in mathematical models used to predict the future health of an ecosystem or ecological reserve?

Summary

In summary, there are numerous fundamental issues central to understanding and predicting climate change and its impacts that fall within the realm of MPS. Such fundamental scientific and mathematical problems need to be solved in order to reduce the uncertainties in future predictions, and hence to develop optimized control, adaptation and mitigation strategies. MPS is uniquely situated to provide the fundamental data, and in addition, to form partnerships across disciplines that will be key to addressing climate change and its impacts.

References

(1) Ezell, M. J.; Johnson, S. N.; Raff, J. D.; Finlayson-Pitts, B. J. *personal communication,* **2009**.
(2) Overpeck, J. T.; Meehl, G. A.; Bony, S.; Easterling, D. R. *Science* **2011**, *331*, 700.
(3) McIntire, T. M.; Ryder, O.; Gassman, P. L.; Zu, Z.; Ghosal, S.; Finlayson-Pitts, B. J. *Atmos Environ* **2010**, *44*, 939.
(4) IPCC "Climate Change 2007: Synthesis Report. Contribution of Working Groups I, II and III to the Fourth Assessment Report of the Intergovernmental Panel on Climate Change," 2007.
(5) Finlayson-Pitts, B. J.; Pitts, J. N., Jr. *Chemistry of the Upper and Lower Atmosphere - Theory, Experiments, and Applications*; Academic Press: San Diego, 2000.
(6) Ramanathan, V.; Ramana, M. V.; Roberts, G.; Kim, D.; Corrigan, C.; Chung, C.; Winker, D. *Nature* **2007**, *448*, 575.
(7) Schwartz, S. E.; Buseck, P. R. *Science* **2000**, *288*, 989.
(8) Warner, J.; Twomey, S. *J. Atmos. Sci.* **1967**, *24*, 704.
(9) Twomey, S. *Atmos. Environ.* **1991**, *25A*, 2435.
(10) Hudson, J. G.; Li, H. *J. Atmos. Sci.* **1995**, *52*, 3031.
(11) Ramanathan, V.; Crutzen, P. J.; Kiehl, J. T.; Rosenfeld, D. *Science* **2001**, *294*, 2119.
(12) Rosenfeld, D. *Science* **2000**, *287*, 1793.
(13) Rudich, Y.; Khersonsky, O.; Rosenfeld, D. *Geophys. Res. Lett.* **2002**, *29*, 17.1
(14) Rosenfeld, D. *Science* **2006**, *312*, 1323.
(15) Rosenfeld, D.; Dai, J.; Yu, X.; Yao, Z. Y.; Xu, X. H.; Yang, X.; Du, C. L. *Science* **2007**, *315*, 1396.
(16) Rosenfeld, D.; Lohmann, U.; Raga, G. B.; O'Dowd, C. D.; Kulmala, M.; Fuzzi, S.; Reissell, A.; Andreae, M. O. *Science* **2008**, *321*, 1309.
(17) Rosenfeld, D.; Lahav, R.; Khain, A.; Pinsky, M. *Science* **2002**, *297*, 1667.
(18) Allan, R. P.; Soden, B. J. *Science* **2008**, *321*, 1481.
(19) Lu, M.-L.; Feingold, G.; Jonsson, H. H.; Chuang, P. Y.; Gates, H.; Flagan, R. C.; Seinfeld, J. H. *J. Geophys. Res* **2008**, *113*, D15201.
(20) Zhang, X.; Zwiers, F. W.; Hegerl, G. C.; Lambert, F. H.; Gillett, N. P.; Solomon, S.; Stott, P. A.; Nozawa, T. *Nature* **2007**, *448*, 461.
(21) Andreae, M. O.; Jones, C. D.; Cox, P. M. *Nature* **2005**, *435*, 1187.

(22) Levy II, H.; Schwarzkopf, D.; Horowitz, L.; Ramaswamy, V.; Findell, K. L. *J. Geophys. Res* **2008**, *113*, D06102.
(23) Rahmstorf, S.; Cazenave, A.; Church, J. A.; Hansen, J. E.; Keeling, R. F.; Parker, D. E.; Somerville, R. C. J. *Science* **2007**, *316*, 709.
(24) Pope, C. A.; Burnett, R. T.; Thun, M. J.; Calle, E. E.; Krewski, D.; Ito, K.; Thurston, G. D. *J. Am. Med. Assoc.* **2002**, *287*, 1132.
(25) Pope III, C. A.; Dockery, D. W. *J. Air & Waste Manage. Assoc.* **2006**, *56*, 709.
(26) Simkhovich, B. Z.; Kleinman, M. T.; Kloner, R. A. *J. Amer. College Cardiol.* **2008**, *52*, 719.
(27) Kleinman, M. T.; Sioutas, C.; Froines, J. R.; Fanning, E.; Hamade, A.; Mendez, L.; Meacher, D.; Oldham, M. *Inhal. Toxicol.* **2007**, *19*, 117.
(28) Firket, J. *Trans. Faraday Soc.* **1936**, *32*, 1191.
(29) Wilkins, E. T. *J. Royal Sanit. Inst.* **1954**, *74*, 1.
(30) Fox, P.; Hendler, J. *Science* **2011**, *331*, 705.
(31) Ramanathan, V.; Justice, C. “Understanding and Responding to Climate Change,” National Academy of Sciences, 2008.