NARSTO Aerosol Workshops

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Overview

- Background
- Workshop Organization
- Summary of Aerosol Processes Workshop
- Summary of Model Applications Workshop
- Future Plans

Background

- Two back-to-back workshops June 26-30 in Boulder, CO
- Purpose: Examine state-of-the-science and research for modeling life cycle of aerosols in air quality management, health effects research, and climate change
- Attendance: More than 50 researchers from Canada, U.S., Mexico, and Europe

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Workshop Organization

- Attendees were provided workshop objectives and specific questions in advance
- Keynote talks to provide background
- Breakout sessions to address specific research issues
- Breakout session recommendations to full group

Aerosol Modeling and Process Evaluation

- Objectives
  - Critical review of past model evaluation activities
  - Assess ability of regional models to simulate aerosol processes and climate effects
  - Review new modeling developments
  - Provide guidance on research needs
  - Discuss PM forecast challenges
  - Discuss opportunities for synergistic research between forecast and climate communities

Aerosol Modeling and Process Evaluation

- Question topics
  - Lessons from past model evaluation activities
  - Current capabilities of high-resolution aerosol models
  - How to conduct model process evaluation

Keynote Presentations

- Steve Ghan, Representing Aerosol Processes in Present and Future Climate Models
- Rohit Mathur, Status and Progress in PM Forecasting
- Stephan Kenne, Evaluating Aerosol Models: Lessons from AeroCom
- Stuart McKeen, Evaluating Aerosol Models: Lessons from ICARTT/NEAQS-2004

Breakout Sessions and Chairs

- New Particle Formation (Peter McMurry)
- Chemistry (Richard Kamens & Sonia Kreidenweis)
- Aerosol/Cloud Interactions and Wet Deposition (Tom Ackerman)
- Emissions, Transport, and Dry Deposition (Chris Doran & Tami Bond)
- PM Forecasting (Rohit Mathur)

Recommendations
New Particle Formation

1. Develop empirical models for NPF rates
2. Modeling studies to assess importance of NPF to climate
3. Develop models for growth rates for freshly nucleated particles
4. Develop methods for measuring trace species that participate in NPF and growth
5. Need collaborative modeling studies and field experiments to evaluate model skill in predicting number distributions

Recommendations Chemistry

1. Need database of SOA formation experiments and SOA precursor emissions for use by modelers
2. Need new analytical techniques for speciating organic aerosols that do not require filter collections, extractions, or harsh preprocessing conditions
3. Design experiments to quantify the role of cloud processing in SOA formation
4. *What should we be measuring? (WTP)*

Recommendations
Aerosol/Cloud Interactions & Deposition

1. Use model simulations and observational data to develop cloud-process parameterizations for regional to global-scale aerosol and climate models
2. Obtain better information on the range in physical and chemical complexity of atmospheric aerosols
3. To gain better understanding of precipitation effects, give priority to characterizing the effects of aerosols on shallow convection and stratus clouds
4. To better characterize the effects of clouds on aerosols, additional research is needed on 1) vertical transport by convection, 2) scavenging and wet deposition of BC, 3) in-cloud chemistry of organic aerosols
5. Increased attention on analysis of past field experiments
6. Additional research on ice nuclei production, ice nucleation, and the the effects of aerosols on these processes

Recommendations
Emissions

1. Need size-resolved information on chemical composition and mixing state of primary emissions at emission
2. Need methodologies for understanding the evolution and formation of aerosols within tens of minutes to a few hours of emission
3. Place priority on developing better emission inventories of primary organic aerosols and precursors (second priority on nitrogen compounds)
4. Regarding source categories, place emphasis on emissions from residential wood combustion, other biofuels, and vegetative burning

Recommendations
Emissions

5. Increased emphasis on integrating in situ measurements of chemical composition with satellite observations
6. North America (NARSTO countries) should be used as a test-bed for developing data-sharing methodologies
7. Significant improvements are needed in the timeliness of emissions inventory data
8. Modeling studies require estimates of future emissions that affect future concentrations of PM

Recommendations Transport and Dry Deposition

1. Studies are needed of vertical transport within and above the boundary layer with particular emphasis on stable conditions in the lower PBL
2. Conduct sensitivity studies on the importance, for climate climate modeling, of improvements in characterizing deposition fluxes for sub-micron aerosols.

Recommendations
PM Forecasting

1. Improve high-resolution met. model, especially vertical mixing in stable conditions and convective clouds. Also need improvements in high-resolution emission inventories (see similar recommendations above)
2. Create an archive of chemical forecast information
3. Additional speciated PM measurements are needed with hourly resolution
4. Conduct an assessment of aerosol loading estimates from regional and global models -- aggregated to common spatial and temporal scales

Recommendations PM Forecasting

5. Four specific process issues require priority attention: 1) heterogeneous NO_3 formation, 2) aqueous SO_4 formation (and understanding discrepancies between measured and modeled total S), 3) representation of carbonaceous mass (including seasonal behavior), 4) representation of fine-coarse interactions
6. Assessment of the feedbacks between chemistry and meteorology (radiative forcing and fluxes)
7. Tools for estimating day-to-day emissions and episodic events
8. Development of a global-scale chemistry forecast model for estimating lateral bcs and research on coupling global and regional forecast models

Applications of PM Models for Source Apportionment and Air Quality Management

- Objectives
  - Assess the performance of emissions-based, chemical transport models in simulating PM concentration, chemical properties, and deposition
  - Assess the performance of receptor and chemical transport models in identifying the sources of primary and secondary PM
  - Provide guidance on observations and methodologies for evaluating the performance of PM models (chemical composition, sources, and discriminating among local, regional and long range sources)
  - Recommend how AQ forecast models might be used to evaluate receptor and chemical transport models

Applications of PM Models for Source Apportionment and Air Quality Management

- Question topics
  - Performance of chemical transport models
  - Source apportionment
  - Model application and performance evaluation

Keynote Presentations

- Jeff Brook, Use and Value of Chemical Transport Models in Regulatory Applications
- Phil Hopke, Receptor Modeling for Source Identification and Apportionment
- Ken Schere, Air Quality Model Evaluation: Forecasting and Retrospectives

Breakout Sessions and Chairs

- Evaluating Air Quality Models for Source Apportionment and Risk Assessment (Jeff Brook)
- Using Receptor and Chemical Transport Models to Improve Air Quality Management (Ted Russell)
- Role of Air Quality Forecasting in Model Evaluation (Ken Schere)

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Recommendations
Evaluating Models for Source Apportionment and Risk Assessment

This session addressed three questions:

1. Given the current (and future data) availabilities and model capabilities, for what applications would you choose receptor models or source-based models?
2. How can we best communicate uncertainty to the various user communities?
3. What research programs or experiments are needed to advance the state-of-the-art in source apportionment and risk assessment?

Limitations of Source-Based and Receptor Models

- Source-based models
  – Coarse spatial resolution
  – Process uncertainties
  – Emission uncertainties
- Receptor models
  – Results can be dominated by local sources
  – Bias is a problem (missing sources will be put somewhere)
  – Difficult to characterize errors
  – Ability to deal with secondary pollutants is questionable
  – Multivariate models will mix sources
  – Source profile information is scarce and expensive
  – Limited ability to provide prognostic information
  – Expensive to obtain high spatial resolution results

Limitations of Source-Based and Receptor Models

- Both models
  - No means for directly evaluating the accuracy of source apportionment results
  - Never enough data

What are the Tradeoffs?

- Source-based models
  - Broader geographical coverage at lower cost
  - Require extensive evaluation, but it is less apparent how to evaluate receptor models
  - Can provide information on processes (how a pollutant got there)
  - Can provide source apportionment information on secondary pollutants
- Receptor models
  - Can provide better temporal response, but limited by data
  - Do not need meteorology

Other Concerns

- How do you reconcile differences between source-based and receptor modeling results?
  - This is an issue requiring additional research
  - However comparing source-based and receptor model results may identify biases or missing sources
- Are there application gaps between the two modeling approaches?
  - At times neither approach may work

How Can We Use Current Models?

Model Type	SIP/AQ Mgnt	Health Studies
Source-based	Yes	Fundamental limitations at present. Best for chronic studies?
CMB	Yes -- for primary emissions	Yes, but does not identify the actor
PMF	Yes -- for primary emissions	Problem with factors not being “pure” (not sure which source is associated with which factor)
UNMIX	Yes -- for primary emissions	Problem with factors not being “pure”
All (and sort out what it means)	No reason to exclude any of the above. Multiple model applications offer insight (but its subjective).	No reason to exclude any of the above. Multiple model applications offer insight (but its subjective).

Communicating Uncertainty

- Policy-makers more interested in confidence in predictions
  - Need to bound the information we provide
  - "Receptor models cannot be more than 100% wrong." (Ron Henry)
  - For SIPs and AQ management, information needs to be provided within a risk framework
- Need to differentiate between error and bias
  - Receptor models not doing a good job on bias
  - Multivariate models can estimate error in the mean, but not day-to-day bias
  - Source-based models need to provide multiple measures of error (skill in predicting concentrations does not equal skill in source apportionment)

What is Needed to Move Forward?

- Accountability as a test of model guidance
- If feasible, a realistic synthetic data set(s) for testing receptor models
- Continued comparisons among different SA models
- Long-term speciation measurements (including organics) and the instruments to do it
- Time series data analysis approaches (especially for source-based models)
- How to characterize source variability
- All the data we can get (don’t eliminate measurements just because they don’t meet an immediate regulatory purpose)
- Communicate clearly (accurate, precise, understandable). Do not confuse source factors with source profiles

Remaining Questions/Issues

- Fundamental limitations regarding
  - Treatment of secondary species by MV approaches
  - Relating source factors to source profiles
  - Spatial and temporal variability (can’t measure everything, everywhere, all the time)
  - Providing uncertainty information to policy makers
- Identify key measurement needs (e.g., source profiles)
- Hybrid models are a good idea, but how do we implement
- How to deal with the bias issue
- Given current and future data availabilities, when do you choose source-based models, receptor models, or both
- What experiments are required to make a leap forward

Role of Air Quality Forecasting in Model Evaluation
(but addressed this issue in passing)

Model Performance Objectives

- Air quality forecasting
  - Capture spatial patterns and temporal evolution of target species
  - 10-20% agreement with observations for forecast metrics
  - Info on PM composition will help inform forecasters
- Health studies
  - Significantly reduce model biases and errors (<20%)
  - Capture spatial and temporal variability
  - Continuous (time-series like) data are needed

Priority Issues

- Data issues and needs
- Characterize model bias and improve model performance
- Improve forecast guidance products
- Refinements to modeling system
- Continuous forecast archive for various applications

Issues Not Covered

- Source emission needs
- Boundary conditions (global chemical models)
- Process issues
- Integrated chemistry/meteorology models

Data Issues

- Standardize data and methods
  - Systematic differences among PM networks and methods
    - Data adjustments to normalize differences among continuous $PM_{2.5}$ instruments
    - Different EC/OC partition methods
    - Evaporative losses from filters
    - Assumptions used to convert organic compounds to mass
  - Measurement method intercomparisons are needed across networks

Data Issues

- Standardize data and methods (cont.)
  - Standardize methods and measurements across networks
    - Consistency in reporting data
    - Enhance data interchangeability across networks
    - Characterize observation errors to help interpret comparisons of models vs. observations
  - Continuous measurements of PM speciation, size distributions and number

Data Issues

- Future recommendations
  - Measurements aloft to provide vertical profiles (lidar, aircraft, satellite)
  - Field studies in different seasons (bias towards summer)
  - Complementary gas-phase measurements (NH_3, precursors for SOA, NO_x, SO_2, O_3, H_2O_2
  - Develop and maintain a network of supersites continuously measuring chemical and physical properties
  - Faster turn-around on PM speciation and size distribution data

Characterize Model Biases

- Assess model performance by season, geographical area, weather regimes and chemical species
- Improve model performance using knowledge gained by model evaluation
- Performance metrics
  - Better metrics for assessing spatial performance (point to grid comparisons are problematic)
  - Temporal variability (timing of build up and dissipation)
  - Improve choice of statistics and indicators (O_3 statistics can't be translated into an expectation for PM)

Improve Model Forecast Products

- Ensemble forecasting
  - Ensemble forecasts out perform forecasts from single realizations
  - Ensembles using different models
  - Ensembles using different realizations
  - Ensemble met forecasts to drive chemical model
- Probabilistic forecasts
- Bias correction
  - Identify systematic biases to correct forecast guidance
  - Update error analysis when model is upgraded
  - Bias correction coefficients should be seasonally dependent

Improve Model Forecast Products

- Chemical data assimilation
  - Satellite column integrated and profile data
  - Other types of profile data (aircraft)
  - Assimilation of surface data
  - Methods development is needed

Refine Modeling System

- Finer spatial resolution
  - Application dependent
  - 4-5 km resolution for urban forecasts
    - Especially for primary PM
    - Grid nesting for major urban areas
    - High resolution does not guarantee better results but is needed for some applications (local “hot spots”, terrain, sea breeze)
- Improved chemistry (trade-off with spatial resolution)

Continuous Forecast Archive

- Need reanalysis or merged products for forecasts and measurements
- Data fusion/data assimilation products could be best product for health studies
- Need strategy for the data archive (what to save)
- Attributes
  - Model data need to be credible for applications
  - Valuable for areas with sparse measurements
  - Valuable for retrospective studies

Future Plans

- Respond to review comments and finalize process workshop report
- Post on website
- Print ~ 100 copies for distribution?
- Finish draft of applications workshop report, obtain peer review, post, and distribute
- Publish summaries in an appropriate journal?