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Draft Summary Report and Next Steps from the Western Meteorological, Emissions, and Air Quality Modeling Workshop

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This workshop was held to discuss research needs to support modeling studies of meteorology, precursor emissions for ozone and primary and secondary particulate matter, air quality modeling for the ozone and PM2.5 NAAQS, and other air quality related values across the Western U.S. Participants included technical air quality modeling staff from Western states, local air agencies, federal land managers, EPA regional offices, and EPA OAQPS. The topics addressed at the workshop fall into four broad categories: emissions inventories, meteorology modeling, air quality modeling and analysis of exceptional events. The meeting participants identified several areas of high priority needs for research or technical support for air quality modeling, and many of these topics involve issues that are unique to the western states. Research needs within each of these categories are summarized below. Meeting participants also identified a near term need for the formation of expert work groups on several of these research and analysis topics, including:

1. Meteorology Modeling
    a. Cold pool meteorology
    b. Over-estimated Rainfall
2. Air Quality Modeling
    a. Background/transported Ozone, including Stratospheric/Free Troposphere/Boundary Layer transport of ozone
    b. Winter Ozone modeling, including heterogeneous and surface chemistry processes
    c. Winter PM2.5 modeling
3. Emissions Data and Emissions Modeling
    a. Oil and Gas, including speciation of VOC
    b. International (Mexico and Canada)
    c. Biogenics
    d. Residential Wood Combustion
    e. Wildland and Agricultural Fire
    f. Nitrogen Deposition and Ammonia/Reduced Nitrogen
4. Analysis of exceptional events and background conditions

Recommended "Next Steps" for topics discussed at the workshop are included. This report will be circulated among meeting participants for additional comments. As noted below, we are seeking conveners for:

- Ongoing workgroups on broad and deep inter-agency topics needing sustained work efforts;
- Conference calls (one or very few) of more limited scope and duration on topics that needs immediate short-term followup; and
- Sessions on all these topics at future regional and/or national modeling workshops for air quality and emissions.

Research and Analysis Topics

1. Meteorology Modeling

a. Cold Pool Meteorology

The failure to appropriately capture wintertime multi-day stagnant air mass conditions (Cold pool) in prognostic meteorological models is precluding photochemical model representation of many different air quality problems: northwest PM2.5 organic carbon, Salt Lake City ammonium nitrate, southwest Wyoming and eastern Utah ozone, and central California ammonium nitrate and organic carbon. Routine application of the prognostic meteorological model WRF with a variety of different physics options, initialization input, and nudging approaches have failed to replicate the stagnant meteorological conditions associated with these air quality problems. New research is needed to develop a boundary layer and land surface scheme to capture multi-day winter-time inversion episodes.

A test-bed for winter cold pool meteorological modeling could be developed using the extensive meteorological measurements taken in Salt Lake City during winter 2011/2012 as part of the Persistent Cold-Air Pool Study (PCAPS) field campaign[1]. The development of a common set of inputs and shared data may allow for further testing of existing WRF options and newly developed approaches.

Next Step: In the near term, a technical workgroup focused on modeling winter-time cold pool events will be formed so members can share experiences and knowledge to best apply existing tools for these situations. A longer-term approach is to work with US EPA/ORD/NCER to establish a STAR grant call for research into developing prognostic meteorological model science to appropriately capture winter cold pool conditions. In a related effort to stimulate longer-term work on this problem, OAQPS has highlighted this research need in a Viewpoint submission to Environmental Science & Technology this summer.

[1] PCAPS website: http://pcaps.utah.edu/

b. Over-Estimated Rainfall

An important prognostic meteorological feature noted is that WRF grossly over-estimates the spatial extent and amount of convective precipitation in the western United States. This feature becomes more pronounced at finer grid resolutions, in particular at 4 km. It is difficult to impossible to replicate elevated summer periods of ozone and PM2.5 if photolysis rates are incorrect or too much precursor mass is removed through wet deposition processes. In addition, the over-estimated rainfall may contribute to degraded model estimates of nitrogen deposition to sensitive regions of the western United States.

A short to near-term approach would be an intensive code review from a model developer to determine if coarse grid features are being appropriately mapped to the finer grids in one and two way nesting WRF simulations. Another short-term approach would be to apply WRF with a complex matrix of physics options, boundary layer schemes, and land-surface models looking for a combination that does not generate excessive convective rainfall to better understand what aspects of the combination of typically used WRF options leads to over-estimated rainfall. It is unclear how either of these approaches would be funded or pursued. In addition, it is not clear if a work-group focusing on this issue would be useful.

Next Step: A conference call or short-term working group should be formed to examine this issue more closely. Recently US EPA has provided precipitation performance for 2007 and 2008 annual 12 km CONUS WRF simulations and do not see the same large precipitation over predictions. More comparison and coordination between US EPA and groups working on WRF modeling in the West may provide an explanation about this discrepancy.

2. Air Quality modeling

a. Background/transported Ozone

Several recent studies have analyzed CASTNet ozone data at rural or remote sites and found large inter-day variability and frequent high ozone levels especially in spring and summer at these sites. Stratospheric intrusion is known to affect surface ozone levels on some days; however, it is difficult to quantify the magnitude and frequency of stratospheric ozone intrusions. Moreover, biogenic precursors and long range transport of ozone and its precursors in the free troposphere might also contribute to variability in background ozone levels and to high ozone levels observed at rural CASTNet sites. There is only very limited ambient monitoring data available to evaluate ozone levels in the free troposphere and as a result, there is significant uncertainty in the appropriate background or transported ozone levels that should be used in SIP modeling for the ozone NAAQS. For regulatory modeling studies that are used to evaluate NAAQS attainment strategies in SIPs, it is especially important that day-to-day variability in ozone transport from the free troposphere to the surface be represented accurately. Errors in background ozone can cause poor model performance for ozone and result in bias in the modeled effectiveness of ozone precursor

control strategies. Thus, there is a need for additional ambient monitoring of ozone profiles in the boundary layer and the free troposphere to represent more accurately background and transported ozone levels in SIP modeling.

Next Step: Form workgroup to review NASA DIAL Pilot Study and WestJumpAQMS Source Apportionment results for transported Ozone. Tie in with EPA "Global Transport" intra-agency working group. Provide a structure that state and federal agencies could use to begin consistent assessment of Ozone exceptional events.

b. Winter Ozone

High winter ozone levels have been observed in the Upper Green Basin, WY since 2005 and high winter ozone levels have also been observed in the Uintah Basin, Utah during the winters of 2009-10 and 2010-11. The cause of winter ozone is believed to be a combination of strong winter temperature inversions, snow cover and large emissions of ozone precursors from the energy sector. Several model sensitivity experiments have shown that photochemical grid models (PGMs) are generally able to simulate elevated winter ozone when emissions of VOC and NOx are adjusted to reflect measured values and when albedo (snow cover) enhanced photolysis rates are characterized. However, it is uncertain whether PGMs can accurately reproduce observed ozone levels for specific episodes and whether the mixing and chemical processes are accurately represented for winter conditions in current PGMs. Modeling of winter ozone requires advances in several of the workgroup areas listed above including: oil and gas emissions; cold pool meteorology; and heterogeneous and surface chemistry processes. Additionally, research needs for photochemical mechanisms were discussed at the workshop. While all current photochemical mechanisms include temperature dependence for key reaction rate constants, it is uncertain whether the temperature dependence of reaction product stoichiometry and photolysis rates are correctly represented. The Carbon Bond gas phase chemical mechanisms are formulated to include temperature dependence in VOC reaction products. The SAPRC chemical mechanism is currently being updated to include similar temperature dependent reactions. The newest version of the Carbon Bond mechanism (CB6) has improvements in aromatic chemistry and other species that should improve representation of winter time gas phase chemistry, but it remains uncertain whether these mechanisms accurately represent gas phase chemistry for the cold weather conditions typical of winter ozone formation. Recent research on the rate constant of OH with NO2 found a reduced rate constant for this reaction, and updating photochemical mechanisms to use the revised rate constant might also improve model performance for radical limited conditions in winter ozone episodes.

Next Step: Review monitoring results from the Uinta Basin 2012 Study and encourage further and more complete analysis of those results. Review results from the WY DEQ winter ozone modeling study that is currently in progress.

c. Winter PM2.5

Episodes of high secondary PM2.5 during winter inversions have been observes in both urban and rural areas in several regions, including the San Joaquin Valley, CA; the Wasatch Front and Cache Valley in Utah, and in Milwaukee and Mayville, WI. In each of these areas the largest component of PM2.5 is ammonium nitrate that is produced by oxidation of NO emissions to form NO2, followed by oxidation to form HNO3, and combination with NH3 to form ammonium nitrate. Key issues in which research is needed to understand formation of winter PM2.5 episodes include cold pool meteorology, heterogeneous and surface chemistry, and winter ozone and oxidant formation.

Next Step: Organize calls to review UT, CA, and WI SIP modeling efforts and methods employed to address these key issues. These issues could then be discussed further at future regional and/or national modeling meetings.

3. Emissions data and emissions modeling

a. Oil and Gas

The Phase III oil and gas inventory includes both point and area source emissions and has been used by both WRAP and US EPA for modeling applications. The Phase III oil and gas inventory will be completed in 2011. Once complete, it provides greater spatial representation of the inventory and includes more sources in each air basin. Several mobile monitoring studies of VOC speciation have been completed or are in progress in CO, WY and UT. Both NOAA and EPA researchers are using mobile labs to detect high methane concentrations near source equipment and then capture a sample for VOC speciation. These studies may provide useful information for improving speciation of oil and gas VOC emissions.

Next Steps: A summary of the data collected and available from the WRAP Phase III project should be prepared. Information about updates to VOC speciation profiles, remaining data gaps, effects of proposed EPA NESHAPs, NSPS and adopted Indian Country minor source permitting and reporting rules, among other issues should be addressed. WGA-WRAP staff will draft this report for broad review, as well as convening calls to review results of NOAA and EPA mobile lab VOC speciation studies.

b. International (Mexico and Canada)

Region 9 indicated that an effort has been completed to update the Mexican emissions inventory (Luisa Molina) to 2005 for the urban centers of Tijuana and Mexicali (no projections to the future). OAQPS is following up with Region 9 contacts to determine what information is available and the scope of the emissions information. There do not seem to be

any current plans to acquire updated emissions information from Canada or if newer data is even available from the 2006 Canadian inventory provided to OAQPS several years ago.

Next Step: US EPA OAQPS followed up with the Region 9 contact and the 2005 emissions for Tijuana and Mexicali are not appropriate for modeling purposes. US EPA OAQPS is currently working with WRAP to generate Mexican emissions that are projected from the 1999 inventory. This issue deserves larger consideration in terms of innovative approaches to generating useful and relevant emissions for both Mexico and Canada.

c. Biogenic Emissions

The WRAP has contracted with ENVIRON and NCAR to develop updated biogenic emissions for the western United States. NCAR will update the MEGAN emissions model with updated landcover/vegetation type data using satellite information from LANDSAT/AWIFS (30 meter resolution). It was determined that the MODIS satellite did not provide the resolution needed to differentiate vegetation types in the western United States. Additionally, higher time resolution estimates (8 day averages) of leaf area index (LAI) will be used as input to the emissions model.. A new version of MEGAN with the updated landcover/plant type information (version 2.1) was released in September 2011. This satellite landcover data may also be used to provide fuel information for the fire emission inventory being developed for the WRAP. A field campaign in northern California (CABERNET) was planned for June 2011 to provide a database to evaluate emissions models on a regional basis.

Next Step: Get update on Western Biogenics study from Tom Moore of WGA and from the appropriate person on the CABERNET study.

d. Residential Wood Combustion Smoke Emissions

Region 10 expressed an interest in finding out how well residential wood combustion smoke emissions are characterized from a variety of combustion sources, fuels, and post-control.

Next Step: Organize a session at upcoming regional and/or national emissions or modeling meetings.

e. Wildland and Agricultural Fire

Regional consistent, complete, and improved fire emissions using transparent methodologies for 2008 across the West will be available from the Deterministic and Empirical Assessment of Smoke's Contribution to Ozone (DEASCO3) study, in early 2013. Potential improvements to the 2008 EPA NEI fire emissions, derived from a separate method, as well as methodological improvements for the 2011 NEI, are under consideration by EPA.

Next Step: Organize a session at upcoming regional and/or national emissions or modeling meetings to assess progress on developing fire emissions inventories and applying them in air quality analyses, including PGMs, exceptional events, and other studies.

f. Nitrogen Deposition and Ammonia/Reduced Nitrogen Emissions

ROMANS I - intensive field campaign in Northern Colorado during April to July 2006.
ROMANS II - intensive field campaign in Northern Colorado during November 2008 to November 2009.

For these study periods, NPS/CIRA has done photochemical modeling of nitrogen deposition in Northern Colorado. Ammonia sources and sinks were characterized using process analysis. CIRA concluded that ammonia deposition in particular needs further study. In addition, large ammonia sources in Northern Colorado including confined animal operations (CAFO) and fertilizer application need improvement in total emissions estimates and temporal allocation to month of the year and hour of the day. It is not clear how well VOC emissions from CAFOs are characterized in the current emission inventory used for modeling purposes. This might be an important regional source of VOC in the western United States. Research by EPA ORD has shown that use of a bi-direction surface flux model in CMAQ can results in improved model performance for NOy and ammonia. Collaboration with EPA ORD with FLM modelers could lead to improved modeling of N deposition and other AQRVs.

Next Step: Organize a session at upcoming regional and/or national emissions or modeling meetings.

4. Analysis of Exceptional Events and Background Concentrations

Examples of exceptional events include episodes of high winds that cause high ambient concentrations of PM from windblown dust; fires that can cause high ambient concentrations of both PM and ozone; and stratospheric intrusion of ozone that can cause high surface level concentrations of ozone. More research is needed in each of these three areas to support air quality regulatory programs. Large uncertainties remain in estimates of PM2.5 and PM10 from windblown dust and it is extremely difficult to model windblown dust in photochemical grid models. More research is needed on fire emissions, both for mass emission rates of primary PM and gasses and for the speciation of primary PM and gasses. Additionally, some data products that can be used in the analysis of possible exceptional events (such as real time forecast model simulations of meteorology and air quality) are not routinely archived and might not be available for subsequent analysis of exceptional events. In some cases the occurrence of exceptional events involve conditions that transcend state and local boundaries, and it would be beneficial to form a workgroup that includes participants from several state and local air agencies to rapidly analyze ambient data and archive key data products for

subsequent analysis. This workgroup could also include researchers from EPA, NASA, NOAA and other federal agencies to assist in the analysis of exceptional events.

Next Step: Form workgroups and leverage states' experience to assess the analysis needs for Windblown Dust, Stratospheric Ozone Intrusion, and Wildfire events. Connect with Ozone Background/Transport Workgroup as identified above, as well as EPA "Global Transport" intra-agency working group. Provide recommendation that state and federal agencies could use to begin to make more consistent assessments of the various types of exceptional events.