Summary of the 4th Peer Review of the CMAQ Model (September 2011):

Recommendations and EPA Response

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June 2011 Review Panel

- Dr. David T. Allen (University of Texas)
- Dr. Praveen Amar (Clean Air Task Force)
- Dr. Nancy J. Brown (Lawrence Berkley National Laboratory)
- Dr. George Kallos (University of Athens)
- Dr. Richard McNider (University of Alabama)
- Dr. Armistead G. Russell (Georgia Tech)
- Dr. William R. Stockwell (Howard University)

Model Evaluation

- *While the group is arguably world leader in the area, there are cases they will need to be **more forward looking** (Support of NAAQS review process: primary & secondary standards; new primary PM.)*
  - Secondary NAAQS
    - Evaluation of modeled sulfur and N (reduced and oxidized) deposition (wet & dry); accounting for biases in modeled precipitation using 2002-2012 model simulations.
  - Primary PM
    - Evaluation of crustal PM constituents
    - Evaluation of single-source modeling approaches (DDM-3D, ISAM, APT, Brute-force)
    - Evaluation of fine-scale WRF-CMAQ applications with field intensives
- *A potential weakness is that they need to examine model evaluation efforts in a **meta (overall) fashion** and need to identify and synthesize what they have learned from all evaluation activities*
  - *Participation in AQMEII*
    - Common evaluation approach for all models – looking at diversity across models
    - Results synthesized and disseminated through journal special issues
  - *Evaluation results are guiding development of linked models across scales (local to hemispheric), media (air-water-land), and issues (AQ-climate)*

Model Evaluation

– *One of their emerging activities, probabilistic evaluation will require more development and application to realize its full potential*

We agree that the area of probabilistic evaluation is important for both regulatory and forecast applications. Examples of our continued efforts:

- Intrinsic uncertainty in models (see poster by Rob Gilliam)
- Ensemble model analyses in AQMEII phase 1 & 2

Chemistry

– *Commended and encouraged the continued development of alternate approaches for chemical mechanisms*

We have tested and included the RACM2 gas-phase chemical mechanism which will be available in CMAQv5.1.

Numerous updates to the CB05 and SAPRC mechanisms to extend their use for emerging applications (e.g., treatment of organic nitrates, linkage with SOA and heterogeneous chemistry)

Active participant in chemical mechanism development community:

- o *Organizing/planning the UC Davis Atmospheric Chemical Mechanisms conference*
- o *Engaged with the researchers in the UK on MCM and condensed version development*
- o *Participated in the recent meetings of NAS Committee on The Future of Atmospheric Chemistry Research*
- o *Working with the EPA STAR program on an future RFP on atmospheric chemical mechanisms for the next generation models*

Chemistry

– *Encourage group to devote more attention to field validation of calculated photolysis rates*

Modeled photolysis rates have been compared with aircraft measurements during field campaigns (ICARTT, DISCOVER-AQ). Clear-sky rates appear to be in reasonable agreement. Challenges are more in assessment of representation of attenuation by clouds (placement and cloudiness) and aerosols (lack of measurements when loading is high).

CMAQv5.1 includes revisions to the treatment of cloud effects on photolysis

- *More details in tomorrow's poster by Bill Hutzell*

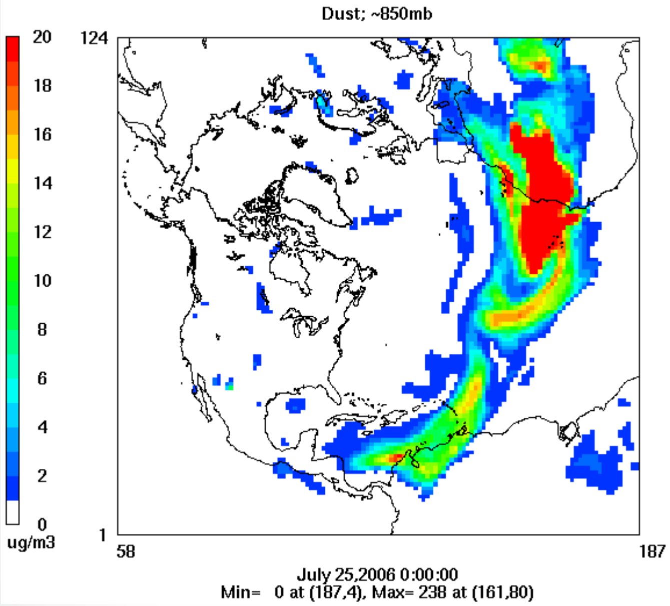
– *Future directions might include incorporation of stratospheric chemistry*

We agree that representation of the stratosphere could be important for emerging applications (e.g., background O_3) and have explored, but not actively pursued incorporation of explicit stratospheric chemistry because (1) current model extent only includes the lower stratosphere, and (2) simulation durations are not long enough to sufficiently represent the key reactions.

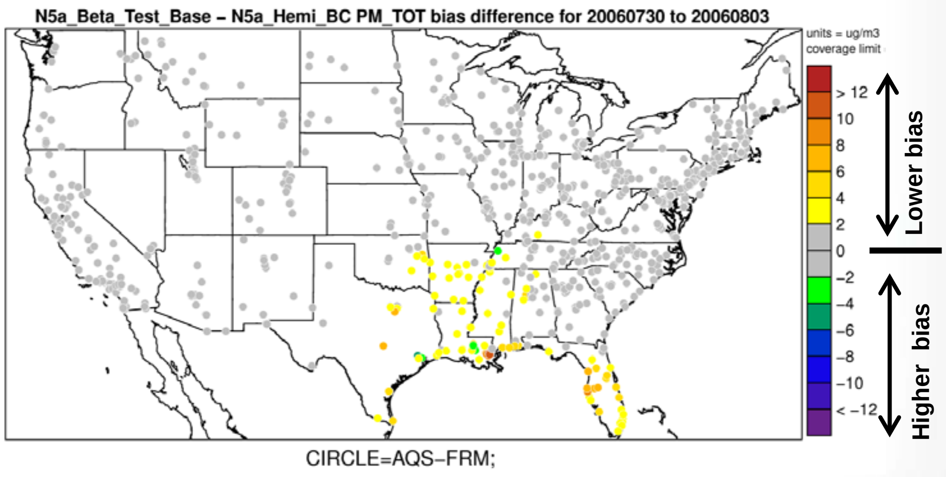
Investigated the use of a potential vorticity scaling for representing impacts of STE on tropospheric O_3 – developing a seasonal and spatially varying scaling.

– *While progress has been significant, need for improvement in: (1) review of soil dust schemes (in limited area models and not GCMs)*

Refinement and testing of the wind-blown dust scheme included in CMAQv5.0, both for continental U.S. and hemispheric applications is an area of continued work. Efforts have also been devoted to improving seasonal estimates of anthropogenic dust in the inventories.



Reduction in bias in simulated surface $PM_{2.5}$



Particulate Matter

– *(2) addition of heterogeneous chemistry processes*

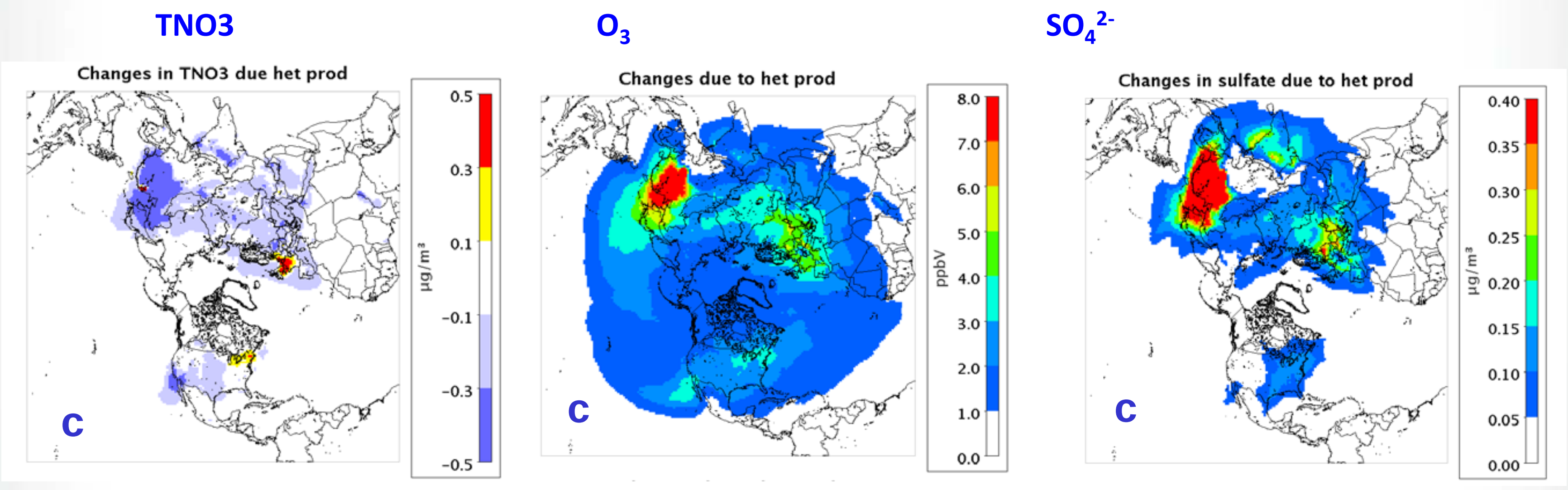
Current model: Uptake of N_2O_5 on aerosols

$N_2O_5(g) + H_2O\ (aq) \rightarrow 2\ HNO_3\ (g)$

When particle contain Cl, uptake of N_2O_5 can also produce $ClNO_2$

$N_2O_5(g) + H_2O\ (aq) + y\ Cl\ (aq) \rightarrow y\ (\ HNO_3(g) + ClNO_2(g)\ ) + 2(1-y)\ HNO_3\ (g)$

Average change in winter-time predictions due to $ClNO_2$ Chemistry



Alters partitioning of reactive nitrogen, impacts oxidant chemistry, and thus impacts production of secondary pollutants (*More tomorrow morning – G. Sarwar & K. Fahey*)

– *(2) addition of heterogeneous chemistry processes*

CMAQv5.1 will also include heterogeneous SOA additions:

- Uptake of IEPOX based on water, sulfate, & acidity in the particle (CB and SAPRC)
- Uptake of MAE (in SAPRC)
- ➢ *More details tomorrow - talk & poster by Havala Pye*

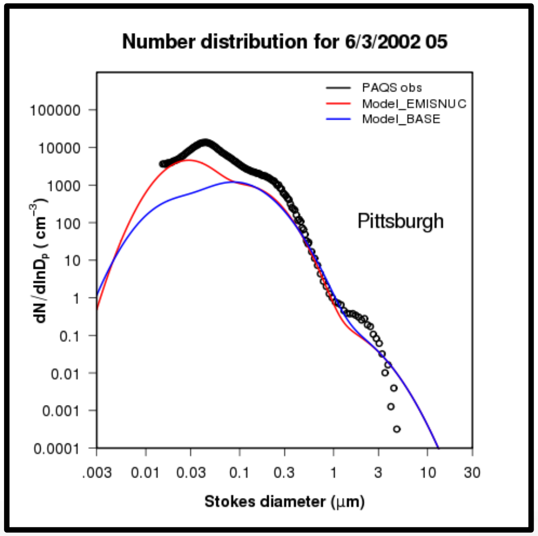
– *(3) Treatment of number density and size distribution (important for met-AQ coupling and aerosol indirect effects)*

CMAQv5.1 incorporates:

(1) corrections to the current binary nucleation scheme (Vehkamaki et al., 2002), and

(2) Update PM emissions modal mass fractions and size distribution based on modern measurements (Ellerman and Covert, 2010)

Compared to Pittsburgh Air Quality Study SMPS measurements, simulated number distributions better represent the observed magnitude and size distribution of particle



Particulate Matter

– ***Identifying and removing sources of bias in sulfate predictions should be a high priority for the Division***

We agree that amongst all PM constituents, predictions of SO_4^{2-} should (and do) have the highest confidence, since SO_2 emissions are well quantified and gas and aqueous formation pathways are well understood.

Bias in SO_4^{2-} predictions stem from a combination of effects: (1) ability of mechanisms to predict OH and H_2O_2 and thus the relative importance of gas vs aqueous pathways; (2) representation of non-precipitating clouds; (3) bias in precip amounts regulating the removal from the atmosphere.

We have examined other plausible pathways for SO_4^{2-} formation to account for the small summertime deficit (e.g., through stabilized Criegee intermediates), but the kinetics of this pathway are still quite uncertain.

Multi-decadal (1990-2010) trends for SO_2 and SO_4^{2-} simulated by the model match well with observations providing confidence in the ability to represent changes in response to changes in emissions and atmospheric dynamics, and thus model inferences drawn on a relative sense.

Expansion of CMAQ to hemispheric scales is now enabling more consistent representation of space and time varying SO_4^{2-} LBCs. DMS chemistry is also being included to complete the troposphericSO_4^{2-} budget.

– ***Continued emphasis on the need to examine problems in a more integrated manner***

We agree that gas-aqueous-aerosol phase connections need to be examined in an integrated manner and have continued to evolve the CMAQ system along those lines

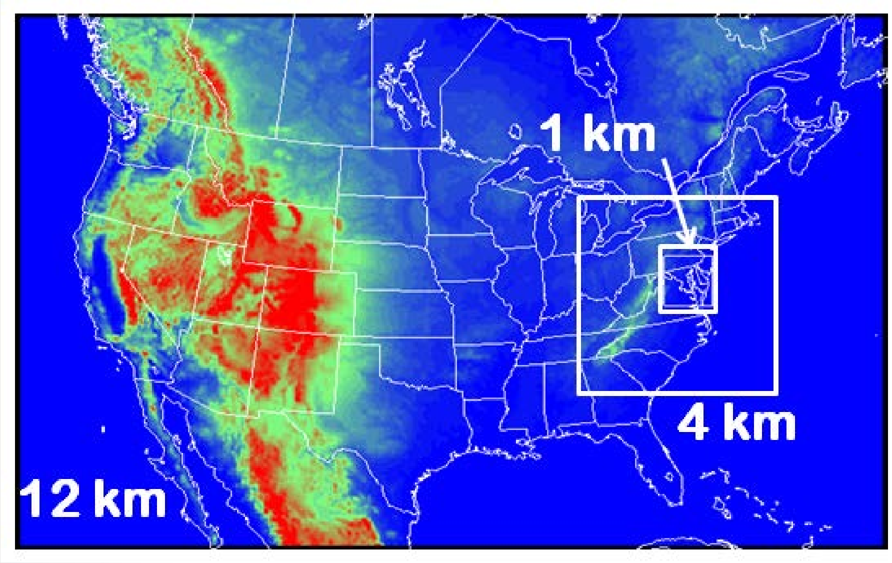
- Example: Poster on *Understanding biogenic and anthropogenic influences in the Isoprene system through improvements in multiple CMAQ components*

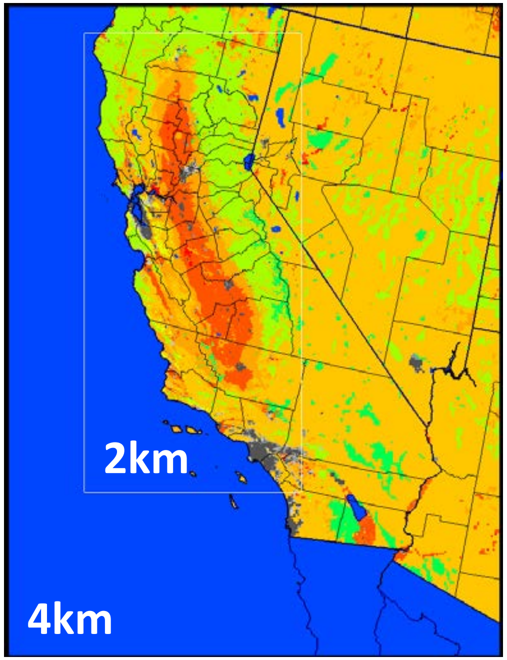
Meteorology Modeling

– *It would be useful to perform more testing at higher resolutions*

Significant effort has been devoted towards improving the representation of meteorology and coupling with the CTM for finer resolution simulations. Model development and evaluation at these fine resolutions (1-4km) have focused on the DISCOVER-AQ field campaigns.

➢ *More details in poster by Wyat Appel (today) and talk by Rob Gilliam (tomorrow)*





Coupled WRF-CMAQ

- *The WRF-CMAQ is efficiently designed. There are question related to its use in other computer cluster configurations*

  The coupled WRF-CMAQ system has been exercised by AMAD on two different clusters at EPA. We have also ported the model to two different DOE machines. We have collaborated with groups in the UK, Greece, and China on WRF-CMAQ applications on different machines. We have not received any specific feedback from the user community on issues related to WRF-CMAQ deployment on different cluster configurations.

- *The coupler is designed to work with one grid configuration and this imposes restrictions on optimal use of WRF capabilities (2-way nesting).*
- *The hemispheric configuration of the coupled model is promising & can be used for LBCs – these features could be enhanced further if fully coupled 2-way nesting for WRF-CMAQ were to be developed.*

  Multiple grids can still be configured for one-way nesting. Our previous work suggests that 2-way nesting poses many fundamental issues related to mass conservation in non-linear chemical flow problems. We thus have not pursued 2-way nesting for non-linear chemistry problems. Nevertheless we acknowledge the need for multiscale modeling for atmospheric problems and instead are exploring alternate approaches for grid refinement that circumvent the issues of discrete boundaries of 2-way nesting (e.g., prototype development of OLAM-Chem; testing of tracer-transport in MPAS).

Coupled WRF-CMAQ

- *Weigh advantages/disadvantages of coupling design and have workshop of experts in the field*
    - Hosted a workshop on integrated meteorology-chemistry modeling
    - Participated in the EuMETCHEM project
    - AQMEII phase 2 focused on coupled models (Poster by Christian Hogrefe)

- *Assess climate change impacts on $PM_{2.5}$*
  We have examined the impact of climate change (based on 2030 projections) on distribution and levels of $PM_{2.5}$. Large uncertainties however exist in projections of natural emissions (wildfires and fugitive dust) in response to climate change and these can influence future regional predictions of $PM_{2.5}$

- *Collaborate with NRMRL on development of realistic future energy scenarios*
  Active collaboration with NRMRL researchers are underway on using MARKAL (and GCAM in future) to estimate emissions associated with future energy scenarios.

- *Benefits could be achieved if SHEDS efforts were more closely linked with CMAQ and the two models could work together*
  Linkages of CMAQ output with the SHEDS exposure model are being discussed with scientists in HEASD. In particular, as starting point, linkage of the 12/4/1km CMAQ predictions for the Baltimore region with the SHEDS model to estimate (and contrast) various exposure metrics (and their sensitivity to spatial resolution) is being explored.

Usefulness of the CMAQ Modeling Program to EPA, States, and Research Community

– *While the effort should not be viewed negatively, OAQPS is using a competing model because CMAQ does not have all capabilities they desire (tools to provide source impacts). If the capability is important and scientifically appropriate, the group should consider adding it. If there are reasons the current approaches are scientifically less well founded, the concern should be clearly communicated.*

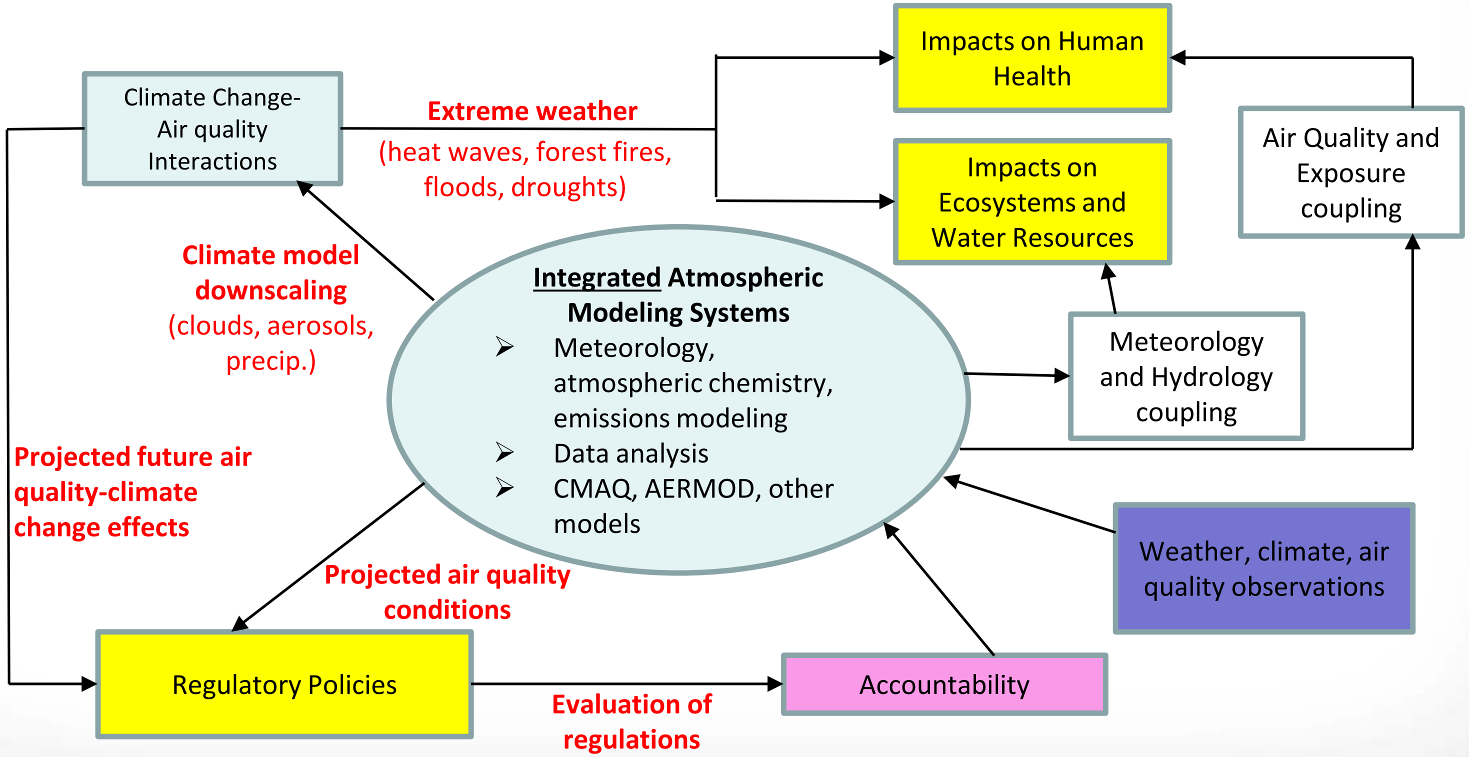
"Backward" attribution and apportionment of non-linearly evolving concentration fields to specific sources (or sectors) pose many numerical and mass conservation challenges. We have worked closely with OAQPS scientists in developing and implementing in CMAQ, source apportionment techniques for PM and O_3. The formulation, assumptions, and applicability of the tools were documented in two peer-reviewed articles. The tools were made available in an interim CMAQ release to the broader community.

- *See poster on Integrated Source Apportionment Method (ISAM) presented by Sergey Napelenok*

Usefulness of the CMAQ Modeling Program to EPA, States, and Research Community

- *In a time of diminishing resources, we recommend that the CMAQ group should continue to develop and enhance the strengths of CMAQ.*
- *Stay focused and not go beyond core mission and competencies*

Though the primary focus of CMAQ applicability within the Agency is on the continental US scale, current and emerging AQ issues require consistent treatment of air pollution from urban to hemispheric scales. Recognizing resource constraints and the growing application needs (e.g., secondary NAAQS and human & ecosystem exposure), we have adopted a "problem-oriented" approach to CMAQ expansions keeping in mind future extensibility and maintenance of the over system.



Usefulness of the CMAQ Modeling Program to EPA, States, and Research Community

– *Develop close collaboration with experts who develop other (media) models*

Extensions of CMAQ to the "One-environment" concept is based on close collaboration with experts of other models that are being connected (e.g., Hydrology, Agriculture, Water Quality). However, some understanding of these systems (space/time scales, first principles vs. calibration) is needed to determine how to link them.

- Additional details in Poster on *CMAQ Applications for Ecosystem and Human Health* presented by Val Garcia

– *Should continue to maintain international collaborations*

We continue to foster and extend international collaborations:

- *Air Quality Model Evaluation International Initiative (AQMEII)*
- *European framework for online integrated air quality and meteorology modelling (EuMETCHEM)*
- *US-UK collaboration on air quality modeling and chemical mechanisms*
- *Collaboration with Tsinghua University on WRF-CMAQ applications in China*
- *Collaboration with IIT-Mumbai on WRF-CMAQ applications in India*
- *Participation on Scientific and organizing committees for many international conferences/workshops*
- *CMAQ applications across the globe provide many opportunities to collaborate and evolve the model for diverse set of conditions*

Additional Recommendations

– *Given team's success in* ***recreating past atmospheres in retrospective studies****, this could be a* ***niche that they could play in global climate arena***
  – We agree that our experience puts us in a unique position for examining past atmospheres.
  – The development of the downscaling methods have used retrospective time periods to verify the fidelity of the techniques.
  – Multi-decadal simulations for 1990-2010 have been conducted to examine the impacts of aerosol radiative effects on atmospheric dynamics and air quality.

➢ *Additional details in Posters on (1) Using CMAQ to Project Impacts of Future Climate Change on Air Quality (Tanya Spero) and (2) Assessment of interactions among tropospheric aerosol, radiative balance, and clouds through examination of their multi-decadal trends (Jia Xing)*

– ***Improve emission inputs to CMAQ model***

Improvement in emission inputs and assessment of their impact on model predictions continues to be an area of active focus:

- Biogenic emissions (*Poster by George Pouliot*)
- Residential wood combustion
- Marine environments: Sea-salt, Halogens (*Posters By Brett Gantt and Golam Sarwar*)
- Emission trends (*Poster by Jia Xing*)