**SOUTHEAST TEXAS PHOTOCHEMICAL MODELING TECHNICAL COMMITTEE**

Meeting Summary
April 25, 2012

H-GAC Offices
3555 Timmons Avenue
Houston, Texas

## Members and Guests Present:

Susan Moore, Arturo Blanco, Isaac Desouza, Dan Cohan, Dan Baker, Marise Textor, Ryan Perna, Melissa Bain, Shelley Whitworth, Graciela Lubertino, Ken Gathright, Jed Anderson, Chris Kite, Jim Smith and Dick Karp, and via telephone, Steve Smith, Judy Bigon, Elizabeth Chism, Liz Hendler, Jim Wilkinson, and Tom Tesche.

All presentations are available on the SETPMTC Web site, http://www.tceq.state.tx.us/implementation/air/airmod/committee/pmtc_set.html.

## SIP Planning and Implementation Update – Lola Brown (TCEQ)

Lola gave an update, which included the following:

- an overview of the TCEQ comments to EPA regarding the proposed Implementation of the 2008 National Ambient Air Quality Standards for Ozone,
- draft dates for 2008 ozone standard SIP development, and
- recent activities related to the TERP program.

Meeting participants asked whether this update would be posted to the SETPMTC web site, and it has been posted. There was also a question about speculating on the base year and attainment year for the 2008 ozone standard SIP. Dick indicated that the base year for emission inventory may be either 2008 or 2011, since they are periodic emission inventory years. However, the final 2011 National Emissions Inventory (NEI) may not be available in time for the expected SIP submission date of August 2015, since modeling would need to be completed a year earlier and initiated at least two years earlier (i.e., summer 2013). Regarding the attainment year, TCEQ staff indicate that it depends on the classification. If the HGB area is classified moderate, then the attainment year would be 2018, but if the area is classified marginal, then the attainment year is 2015. In addition, TCEQ staff indicated that if the area is classified as marginal, no attainment demonstration (i.e., modeling) is required as part of the SIP submission.

For questions or more information, please contact Lola at lola.brown@tceq.texas.gov.

## H-GAC Air Quality Issues – Graciela Lubertino Ph.D. (H-GAC)

Graciela presented information on the recent update (i.e, 2012 amendment) to the 2035 Regional Transportation Plan (RTP) update, in particular, revisions to the 2011-2014 and 2013-2016 Transportation Improvement Projects (TIPs). The conformity analysis (MOBILE6.2) associated with the amendment indicated that for the 2018 future year, on-road mobile source emissions of $NO_X$ and VOC are less than the SIP 2018 MVEB. Asked about the notable reduction in projected VMT, Graciela responded that a revised HPMS adjustment factor (i.e., ~ 0.9) and application of feedback loops to account for congestion have reduced the future projection of VMT.

For questions or more information, please contact Graciela at graciela.lubertino@h-gac.com.

## Factors Influencing Ozone-Precursor Response in Texas Attainment Modeling (AQRP-008) – Dan Cohan, Ph.D. (Rice University)

As Dan explained, this project was motivated by the concern that while air quality models, including their various components and inputs, have a degree of uncertainty, the modeling results are used in a deterministic manner (i.e., without consideration of the uncertainty) to test for control strategy selection and attainment. Both the test for control strategy selection and attainment depend on the modeled ozone to precursor sensitivity, that is, the change in ozone concentrations to the change in precursor emissions (i.e., $NO_X$ and VOC). The goal of the project was to investigate approaches for characterizing the uncertainty in the modeled ozone sensitivity to changes in emissions.

Uncertainties in the model's components (structural uncertainty) and the inputs (parametric uncertainty) were estimated by varying these features using typical alternatives. For example, after an initial evaluation of several of the modeling components, the structural uncertainty was estimated using biogenic emissions derived from two different models (i.e., GloBEIS and MEGAN), two different chemical mechanisms (CB05 and CB6) and two different deposition schemes (RADM and Zhang). For the parametric uncertainty, an initial evaluation identified the parametric values from the boundary conditions and reaction rate constants as having the most influence on ozone concentration and ozone to precursor sensitivity. Therefore the parametric uncertainty was estimated by using boundary condition values derived from two different global models (MOZART and GEOS-Chem) and a series of percentages of the rate constant for the reaction, $NO_2 + OH => HNO_3$.

As Dan further explained, using these sets of alternate structural and parametric scenarios, a Monte Carlo analysis was conducted with a reduced form of the model which runs fast enough to accommodate the thousands of simulations needed to generate the variability (uncertainty) in the results (i.e., ozone concentrations and ozone to precursor sensitivities). Additionally Bayesian statistical constraints were applied, based on modeling performance in simulating observed concentrations of ozone, to weight the likelihood of the Monte Carlo simulated results. Two Bayesian approaches were used to develop weighting factors for the probability distributions. One approach weighted the likelihood at selected sites based on the model performance for days with

high monitored eight-hour ozone concentrations (i.e., > 70 ppb). The other approach weighted the likelihood based on the model performance for days with high monitored eight-hour ozone concentrations for the average of selected sites. A third non-Bayesian approach weighted the likelihood based on the inverse of the sum of the modeling performance metrics: MNB, MNGE and UPA. These weighted results yield probability distributions for predicting the best estimates of ozone to precursor sensitivities.

During Dan's presentation, he was asked about the monitors used in the analysis for DFW, in particular, whether the Kaufman monitor, as depicted on slide 22, was one of the selected monitors. Dan responded that the three monitors selected for the DFW analysis were Denton, Eagle Mt. Lake and Keller, which are the monitors with the highest eight-hour ozone design values. The Kaufman monitor was not used and the slide should have depicted the Keller monitor instead.

Dan was also asked about using ozone to precursor sensitivities based on monitored data (e.g., weekday versus weekend) for weighting the likelihood of Bayesian Monte Carlo simulations instead of the monitored ozone concentrations. Dan responded that using ozone to precursor sensitivity, which could be derived from weekday versus weekend monitored data, would be advantageous and it can provide a target estimate for the modeled sensitivities. However, unlike ozone concentrations, which are routinely measured at many monitors, ozone to precursor sensitivities are not routinely measured.

Dan also responded to a comment about the chemical mechanism being a key structural component and a suggestion that a better estimate of uncertainty would be achieved using the Carbon Bond (CB) and the SAPRC mechanisms as opposed to different version of the CB mechanism (i.e., CB05 and CB6). In particular, it was mentioned that in comparisons between SAPRC and CB mechanisms, SAPRC often results in larger ozone to precursor sensitivities. Dan agreed that SAPRC does use a different scheme, which may account for difference between ozone to precursor sensitivities, although CB6 includes a number of major changes from CB05.

Regarding the results of the ozone sensitivity to anthropogenic emissions, particularly $NO_X$, Dan was asked about the mobile emissions factor model (i.e., MOBILE6 or MOVES) used, since MOVES estimates notably larger $NO_X$ emissions for the same amount of VMT. Dan responded that these results were based on modeling with MOBILE6, but that modeling using MOVES would be expected to shift the distribution of the ozone to $NO_X$ sensitivity.

Dan was also asked how different the ozone to anthropogenic emission sensitivities would be for the HGB area relative to the DFW area. Dan responded that as opposed to the DFW area where ozone production is almost always $NO_X$ limited, the HGB area is much more transitional between $NO_X$ limited and VOC limited in both time of day and spatially.

For questions or more information, please contact Dan at cohan@rice.edu.

**MOVES2010a Update of the 2006 and 2018 On-Road Emission Inventories for Houston/Galveston/Brazoria (HGB) – Chris Kite (TCEQ)**

Chris presented an update on the baseline (2006) and attainment year (2018) on-road mobile source emissions modeling with MOVES2010a. Of particular interest are the SIP quality on-road, link-based emissions for the HGB area. Chris presented a number of tables and charts comparing the MOBILE6.2 and MOVES2010a emission estimates. He then summarized the MOVES2010a estimates arrayed by emission process (e.g., exhaust, evaporative), vehicle type (e.g., passenger cars, heavy-duty trucks), day type (e.g., weekday, Sunday) and county.

During Chris' presentation, he was asked about the MOVES2010a feature that separates $NO_X$ emissions into the NO and $NO_2$ components, in particular, whether NO is estimated as NO or $NO_2$, the latter of which is the convention for reporting mass emissions of $NO_X$. Chris responded that since MOVES2010a calculates $NO_X$ as the sum of NO + $NO_2$, it uses the molecular weight of $NO_2$ (46) for reporting mass emissions in units such as tons per day.

Chris was also asked about the impact on emissions due to the change in the fuel type between the 2006 base year and the 2018 future year, in particular, the use of ethanol and biodiesel. Chris responded that very little ethanol was in use in 2006, but 2008 was a significant phase-in year for ethanol in Texas. Increased nationwide use of ethanol and biodiesel is occurring in order to meet federal requirements for renewable fuel use, so both fuel types are expected to be used in 2018.

Chris also responded to a comment about the peak manufacturing and warehousing of 2006 heavy-duty diesel engines just before tighter 2007 standards were introduced, which could delay the fleet turnover with newer less polluting diesel engines. Chris indicated that although the older model diesel engines were stock-piled, the delay in the fleet turnover is not expected to be extensive.

Chris was also asked whether the March 2010 attainment modeling, which used MOBILE6.2 and thus lower on-road $NO_X$ emissions than if MOVES2010a had been used, means the attainment modeling would have over-estimated emissions from stationary sources. Chris responded that for attainment, the modeling is used in a relative sense, implying that, to a certain extent, over- or under-estimates in the base and future modeling ratio out. Other TCEQ staff explained that the total modeled emissions using MOVES2010a have increased above the total emissions in the March 2010 attainment modeling. Additionally, this emissions increase has increased the 2018 projected ozone design value. However, the increase in the design value occurred predominantly at the Bayland Park monitor rather than the Deer Park monitor, which was the projected design value monitor in the March 2010 attainment modeling. The 2018 projected ozone design value increase associated with MOVES2010a makes Bayland Park the design value monitor with a value of 87 ppb which is the EPA upper-bound threshold for weight-of-evidence applicability.

Chris was also asked how revocation of the 1997 ozone standard would affect the applicability of the MVEB for conformity, since the budget is based upon compliance

with the 1997 ozone standard. Chris and the other TCEQ staff indicated that, as they understood the conformity rules, the revocation of the 1997 standard would not negate the use of the latest EPA-approved MVEB for conformity.

For questions or more information, please contact Chris at chris.kite@tceq.texas.gov.

**Characterization of Gulf Background Ozone Concentrations - Jim Smith, Ph.D. (TCEQ)**

Jim's presentation investigates the CAMx modeling issue of over-prediction of ozone concentrations in ambient air arriving from the Gulf of Mexico as measured at coastal monitoring sites, such as Galveston (GALC, CAMS 1034). Jim used HYSPLIT model-created 48-hour back trajectories ending at GALC for every other hour of every day of the May to September ozone season for the five year period, 2007 to 2011, a total of 9180 trajectories for which there was sufficient data available to simulate 8792 trajectories. Using a Potential Source Contribution Function (PSCF) type analysis, which assigned hourly ozone concentrations measured at GALC for the terminal hour of the back trajectory to each trajectory point, the median ozone concentration was determined for all trajectory points within each grid cell of an overlaid 36 km by 36 km domain. This analysis showed that winds from the Yucatan over the western segment of the Gulf transport ambient air with ozone concentrations ranging from 10 to 20 ppb, and winds from Cuba over the mid and eastern segments of the Gulf transport ambient air with ozone concentrations ranging from 15 to 25 ppb.

During the presentation, Jim responded to a comment concerning the use of $O_X$ (i.e., $O_3$ + $NO_2$) when comparing the modeled versus monitored values, but using $O_3$ for the HYSPLIT-PSCF analysis. As Jim explained, during periods with sustained south-southeasterly winds, the ambient air has very little, if any, measurable $NO_2$ concentration.

Next Jim presented the results of applying a cluster analysis that incorporated both the horizontal and vertical transport components associated with the back trajectories. This helped to further distinguish wind regimes transporting ambient air with high and low ozone concentrations. For example, ozone concentrations in ambient air transported over the Gulf were slightly lower for trajectories emanating from higher altitudes (e.g., above the daytime mixed layer).

For questions or more information, please contact Jim at jim.smith@tceq.texas.gov.

**Reactive Plume Modeling to Investigate NOx Reactions and Transport in Nighttime Plumes and Impact on Next-day Ozone (AQRP-020) – Dick Karp, (TCEQ)**

Dick presented a review and summary of the AQRP study of nighttime $NO_X$ chemistry in two distinctly different coal-fired power plant plumes sampled during TexAQS II with the NOAA P-3 aircraft. The Oklaunion power plant is located in north Texas in an area with very few other $NO_X$ emission sources, while the Parish power plant is located southwest and adjacent to the Houston metropolitan area, a region with numerous $NO_X$

emission sources. In addition, the $NO_X$ emission factors for the two power plants are an order of magnitude different.

As Dick showed, a review of the aircraft sampling (in particular, for the Oklaunion plume) indicates the plume had limited vertical extent and most likely the horizontal transects did not pass through the plume center, but were well above or below the center. Since plume models are configured to simulate the concentration distribution through the center of the plume, using the transect data as representative of the plume center may be questionable. In fact as Dick's review indicated, both the plume modeling with SCICHEM and CAMx were unable to adequately replicate the plume transects, even when the modeling configurations were significantly altered.

In comparing the SCICHEM modeling results with the aircraft measured $N_2O_5$ across the plume transects, Dick was asked about the asymmetry of the modeled distribution of concentrations. Dick responded that this asymmetrical feature of the SCICHEM modeling was not addressed in the report. It was noted that the aircraft transects were not exactly perpendicular to the wind direction, which may account for the asymmetry.

Also, during the presentation of the CAMx modeling with PiGs, Dick was asked about the criteria used in the modeling to determine when the constituents within the PiGs (e.g., $NO_2$) were mixed (i.e., dumped) into the grid cells. Dick responded that as he understood the modeling criteria, PiG puffs were dumped when the horizontal area of the puff exceeded a certain percentage of the grid cell area, such as 75%.

During a discussion concerning the production of $N_2O_5$ within a plume being dependent on whether ambient ozone or plume NO concentrations are in excess, it was mentioned that for the aircraft sampling during the night of October 11- 12, 2006, of the Parish power plant plume, the ambient ozone concentration outside the plume (e.g., background) was approximately 50 ppb, with a southerly wind. This level of ozone seems a little high, since as Jim Smith's presentation showed, a 15 to 25 ppb ambient ozone concentration is more typical of a southerly wind and therefore the notable amount of $N_2O_5$ measured in the Parish power plant plume may not be typical.

For questions or more information, contact Dick Karp at dick.karp@tceq.texas.gov.

**Meeting Schedule and Agenda Topics 2012**

The meeting participants discussed setting a date for a meeting in June, during which it was mentioned that there were known conflicts for all but the last week of June. Dick indicated he would work with Graciela to identify candidate days for a June 2012 meeting. Once candidate days are identified, Dick indicated he would poll the members to see if there is a preferred date.

Dick indicated he was planning to schedule presentations for other AQRP projects for the June meeting, such as the SOF and DOAS ambient air measurement project in southeast Texas during the spring of 2011. An update on the NASA Discover-AQ project, scheduled for the Houston area in late summer of 2013, was also mentioned as a topic for the June meeting. Additionally, Dick mentioned that by the end of June, the

TCEQ may be able share some of the CAMx modeling being conducted for the MOVES MVEB replacement SIP revision.

The meeting was adjourned.