SOUTHEAST TEXAS PHOTOCHEMICAL MODELING TECHNICAL REVIEW COMMITTEE

Meeting Summary
December 12, 2007

H-GAC Offices
3555 Timmons Avenue
Houston, Texas

Members & Guests Present:

John Dege, Thomas Ho, Ken Gathright, Jan Stavinoha, Graciela Lubertino, Christine Smith, Judy Bigon, Rohit Sharma, Dan Baker, Dan Cohen, Karl Pebble, Al Hendler, Rebecca Rentz, Ashley Forbes, Lola Brown, Jim Smith, and Dick Karp, and Liz Hendler, Steve Kilpatrick, Erik Snyder and Tom Tesche via telephone.

SIP Planning & Implementation Update – Lola Brown (TCEQ)

Lola gave a brief verbal update. She provided TCEQ web site addresses where stakeholders can access information on SIP-related activities and issues:
http://www.tceq.state.tx.us/implementation/air/sip/Hottop.html &
http://www.tceq.state.tx.us/implementation/air/sip/hgb.html &
http://www.tceq.state.tx.us/implementation/air/sip/bpa.html.
Lola also provided information on how to get e-mail updates by signing up on the agency's web site.

Regarding HGB activities, Lola indicated that TCEQ is conducting internal research and analysis of potential control strategies for the HGB attainment demonstration. In response to questions, Ashley Forbes indicated she is the contact for stationary source control strategies and Donna Huff is the contact for mobile source control strategies.

Lola also discussed the latest activities regarding the BPA SIP. Although the eight-hour ozone 2006 design value indicated BPA did not achieve monitored attainment of the standard, as required for a marginal nonattainment area, the current 2007 design value shows that the area is monitoring attainment of the standard. A *Federal Register* notice was published October 30, 2007, that proposes to bump up the classification to moderate. However, since the area is currently monitoring attainment, the EPA anticipates publishing another notice suspending the moderate SIP requirements. The SIP requirements may be suspended until the area does not monitor attainment in 2008 or until designated as attainment and a maintenance plan is put into place. Lola also stated that the options are currently under review by TCEQ.

H-GAC Update – Graciela Lubertino, PhD (H-GAC)

Dr. Graciela Lubertino gave a brief verbal update. She reported that H-GAC has not yet received a notice-to-proceed from TCEQ regarding the project to identify new control measures. Although TCEQ staff has indicated the project has been approved by TCEQ management.

Graciela also indicated that an amendment to the conformity analyses has been approved by both TCEQ and EPA and H-GAC is waiting for approval from FHWA. Also another amendment is going to be processed to correct an error in the metro routes. A question was raised as to whether the error in metro routes affects the on-road emission inventories developed by TTI for the next SIP. The consensus seemed to be that the error would not affect the TTI developed emission inventories.

Graciela also reported that H-GAC had just completed a study of fuel economy. This study indicates that approximately 5 million gallon of fuel (gasoline and diesel) is consumed daily in just Harris County, and that gasoline consumption is about four times that of diesel. There was some discussion of using the data from the study to compare with on-road emissions. A question was asked about how diesel consumption was determined, since diesel fuel sold for use in long-haul trucks would not all get consumed within the HGB area and visa-versa for long-haul trucks entering the area. Graciela stated that EPA national data for fuel consumption was used, because regional data is not based upon fuel consumption, but instead is based upon evenly distributed tax revenue.

EPA SIP Related Update – Erik Snyder (EPA)

Erik gave a brief verbal update. The appeals court handling the litigation on the HGB 1-hour SIP has contacted the parties involved about scheduling to hear oral arguments the week of January 28, 2008. This litigation, in part, involves the HECT and MECT rules in the December 2004 SIP, which EPA approved in August 2006.

Erik also reported that the draft of the Federal Register Notice for the reclassification request is currently being reviewed and EPA is still hopeful that it will be published by the end of the year.

On the national level, Erik reported that there are still a number of areas that have not submitted their 8-hour ozone SIPs, which were due June 15, 2007. Nonattainment areas included within this group are the LADCO states, California and most of the states comprising the Philadelphia area. Erik indicated that EPA has not yet decided how to handle failure to submit, but EPA will need to act soon. Erik reported that LADCO has indicated they will be submitting an attainment SIP in March 2008, which uses 2005 base case modeling. In addition, California has apparently indicated they will be submitting their SIP in a couple of months, which will include a request for reclassification and a modeling demonstration for the reclassified attainment date.

Erik indicated EPA is working on the comments received on the proposed new 8-hour ozone standard(s) and expects to publish the final in the Federal Register in March 2008.

2005 Base Case Model Performance Update, Ozone & Ozone Precursors– Dick Karp (TCEQ)

Dick presented statistical and graphical model performance evaluations for the most recent round (regular3) of CAMx modeling for the 2005 episodes. (Note: Dick's presentation is available on the SETPMTC web-site: http://www.tceq.state.tx.us/implementation/air/airmod/committee/pmtc_set.html). The major differences in the modeling inputs from the previous round (regular1) of CAMx modeling for the 2005 episodes are the episode-specific on-road mobile source emissions and the use of daily geographically varying sea-surface temperatures in the meteorological modeling and the subsequent effect on the meteorological input parameters. Another noteworthy change is modeling with a nested 2km X 2km gridded domain.

In particular, Dick presented statistical model performance evaluations for measured versus modeled peak 1-hour and 8-hour ozone concentrations, and relative bias and relative error for 1-hour ozone concentrations greater than 60ppb and for daily maximum 8-hour ozone concentrations. Graphical model performance evaluations consisted of time-series of 1-hour ozone, nitrogen oxide and nitrogen dioxide, and scatter-plots of measured versus modeled HRVOC CB05 species for selected monitoring sites. (Note: the hourly ozone animations were not presented due to time constraints.)

Questions and comments that arose during Dick's presentation included whether chlorine chemistry is included in the CB05 mechanism; the dichotomy between the relative bias and relative error for 1-hour ozone concentrations and the relative bias and relative error for the daily maximum 8-hour ozone concentrations; distinguishing between daytime versus nighttime measured versus modeled HRVOC CB05 species in the scatter-plots; and adding quantile-quantile plots of the HRVOC CB05 species. Dick responded that chlorine chemistry is not included in the current CB05 chemical mechanism and without a more definitive emissions inventory for reactive chlorine compounds, it may not be that useful to include the chlorine chemistry in the CB05 mechanism. Dick acknowledged that there is a noteworthy difference between the relative bias and relative error for 1-hour ozone concentrations which are based upon all hourly pairs of monitored and modeled concentrations ($\geq$ 60ppb) at all sites, and just the maximum daily 8-hour pairs of monitored and modeled concentrations at all sites. As Dick explained, the relative bias and relative error for 1-hour ozone concentrations provides the best set of model performance statistics, as opposed to the comparable 8-hour moving average ozone concentrations (which have been determined but were not included in the presentation), while the relative bias and relative error for the daily maximum 8-hour ozone concentrations relate to the use of these modeling results in the calculation of the denominator of the relative reduction factor and the subsequent estimate of the future ozone design value. Dick pointed out instances (e.g., May 23, 2005) where the relative bias for the daily maximum 8-hour ozone concentrations appear to be rather acceptable (e.g., < 5%), while the relative bias of the 1-hour ozone concentrations are outside the bounds of EPA's recommended level (i.e., > $\pm$ 20%). These instances suggest that the daily maximum 8-hour ozone concentrations are being suitably replicated, but possibly for the wrong reasons. Dick acknowledged that discriminating between daytime versus nighttime measured versus modeled HRVOC CB05 species in the scatter-plots; and adding quantile-quantile plots of the HRVOC CB05 species were good suggestions and TCEQ will likely add them to the model performance evaluations.

Dick summarized the current model performance for the three 2005 episodes noting that two of the episodes notably under-predict monitored 1-hour ozone, while the other episode generally over-predicts the monitored 1-hour ozone. Oxides of nitrogen are not well replicated, with a general over-prediction of nitrogen dioxide. Monitored versus modeled correlations for ethene (CB05 ETH) are fairly good except at the higher concentrations (e.g., > 10ppb-C), while both CB05 species, OLE and IOLE, are generally under-predicted, especially IOLE.

Reconciling Reported VOC Emissions with Ambient Measurements –Jim Smith, Ph.D., (TCEQ)

Jim's presentation explained a procedure TCEQ is investigating with regard to reconciling the reported emission of the HRVOC species with ambient measurements from the Automatic Gas Chromatographs (auto-GC's). (Note: Jim's presentation is available on the SETPMTC web-site: http://www.tceq.state.tx.us/implementation/air/airmod/committee/pmtc_set.html).

As Jim indicated, since 2003, the HGB area has had an extensive network of auto-GC's, which measure ambient concentrations of many hydrocarbon species, including the HRVOCs. In 2005 and 2006, twelve sites operated in Harris (8), Galveston (1), and Brazoria (3) counties. Jim's presentation focused on the ambient concentrations of HRVOCs measured in 2005 and the reported emissions of HRVOCs reported in 2005. Jim pointed out that emission rates (lbs/hr) and ambient concentrations (ppb) are not directly comparable, and models, which also need meteorological inputs are required to transform emission rates of gaseous constituent into estimated constituent concentrations, more comparable with measured ambient constituent concentrations. This, in part, is what CAMx does, although it is impractical to run CAMx for numerous time periods (e.g., thousand/year) at a relatively high resolution, so the simpler Industrial Source Complex (ISC) air quality model was selected, which can be run hundreds of times in comparison to a single run of CAMx.

As Jim pointed point, the ISC model imposes some constraints, most notable the assumptions of "straight-line" winds and no chemical reactivity. To address the assumption of straight-line winds, ISC was only run for hours during 2005 for which the wind direction remained relatively constant for at least six consecutive hours. Although ISC can be run with a decay feature to approximate chemical reactivity, it was not used in this initial analysis. As was pointed out, for the HRVOCs, which are highly reactive, this would mean the ISC modeled HRVOCs should be larger than the measured ambient HRVOCs, presuming that the inventory of HRVOC sources adequately represents the HRVOCs being emitted.

As an example of the use of the ISC modeling, Jim presented a graphical display of pollution-roses, with 10-degree directional increments, comparing the ambient measured and ISC-modeled median propylene concentrations for each of seven auto-GCs over-laid on a propylene emissions map of the Houston Ship Channel. In general, the pollution-roses comparing the measured and modeled HRVOC concentrations show a notable under-prediction by the model, suggesting that the reported emissions of HRVOCs are too low, although the degree of under-reporting suggested varies by the HRVOC species. While the pollution-roses provide an indication of the directions from which HRVOCs are notably too low, they do not indicate a distance away from the monitor, and therefore can not identify a likely location for missing HRVOC emissions.

To address the need to locate likely source regions of missing HRVOCs, the Potential Source Contribution Function (PSCF) was selected. The PSCF technique has typically been used (Xie & Berkowitz, 2005) to locate source regions associated with relatively high (e.g., 75th percentile) pollutant (e.g., HRVOCs) concentrations. In general, the PSCF analysis associates a back trajectory from a monitor with the measured concentration at the monitor. For the PSCF analysis, back trajectory locations were determined at 5-minute intervals, so each back trajectory consisted of 72 points. By over-laying the 72 points of each back trajectory on a 2km by 2km gridded domain, the number of back trajectories passing through the various grids, as well as the number associated with high concentrations can be determined. The PSCF value for a grid is the ratio of the number of back trajectory points in the grid associated with relatively high concentrations to the total number of back trajectory points in the grid. So grids with high ratios are an indication of areas most likely to have contributed to the relatively high concentrations.

As an example of the results from PSCF analysis, Jim presented a graphical display of the gridded PSCF values for propylene at the Lynchburg Ferry (LYNF) auto-CG monitor over-laid on an emissions map of the 2km by 2km gridded domain. In this example, the "high concentration" was defined as the 75th percentile value, data for both 2005 and 2006 were combined, and the back trajectories were not limited to just the "straight-line" 6-hour back trajectories. (Note: the PSCF analysis does not require straight-line winds as does the ISC analysis). Jim pointed out that while the PSCF analysis for LYNF identifies know emission source areas as likely (i.e., having high PSCF values) contributors to "high" measured concentrations, it shows "tails" (i.e., grids with high PSCF values) that extend beyond the emission source areas, which are considered artifacts of the procedure. Next Jim presented a graphical display of the gridded PSCF values based upon combining the analysis for all the monitors. By combining the PSCF analysis for all the monitors, the identification of likely emission source areas can be more specifically indicated and the "tailing' can be reduced. However, the PSCF analysis does not quantify how much the emissions may be under or over-estimated.

In an effort to try to meld the results from the ISC modeling and the PSCF analysis, Jim presented an alternative to the typical PSCF analysis discussed above. In the alternative PSCF analysis, entitled PSCF Type 2, rather than counting the number of back trajectory points within each grid, the concentration values associated with the back trajectory points were tallied. Jim presented a graphical display of the PSCF Type 2 results, depicted by the median of the concentrations tallied within each grid. These results

(i.e., medians) are for the combination of all monitors using the "straight-line" back trajectories and associated ambient propylene concentrations used in the ISC modeling analysis. In the graphical display, the median ambient propylene concentrations were over-laid on an emissions map of the 2km by 2km gridded domain, which generally shows the grids with higher median values to be coincident with the locations of reported propylene emissions. The PSCF Type 2 analysis was applied a second time, again using the "straight-line" back trajectories from the ISC modeling, but this time with the ISC-modeled propylene concentrations, rather than the ambient measured propylene concentrations. Jim presented a similar graphical display of the PSCF Type 2 results, depicted by the median of the modeled concentrations tallied within each grid.

In general, the PSCF Type 2 analysis, using the ISC-modeled concentrations, yields a smaller median concentration for the various grids, than the PSCF Type 2 analysis using the ambient measured concentrations (i.e., suggesting that the reported emissions of HRVOCs are too low). Taking the ratio by grid cell of the medians, i.e., the ambient measured HRVOCs based medians to the ISC-modeled HRVOCs based medians, provides an emission reconciliation factor (ERF) for each grid cell. Jim presented a series of graphical displays of the gridded ERF values for various HRVOCs over-laid on an emissions map of the 2km by 2km domain. As Jim discussed, applying the ERF to the reported emissions can be approached in at least a couple of ways. For example the ERF can be applied on a grid by grid basis to all the sources with in the grids, or the ERF can be applied on a domain-wide basis (e.g., the 8-county area) assuming all the emission reconciliation is due to only one source category (e.g., point sources). Jim presented a table of ERFs for various HRVOCs developed as a constant multiplier for point sources within the 8-county HGB area. These area-wide constant ERFs applicable to point sources of HRVOCs ranged from 1.52 for 1,3-butadiene to 3.66 for propylene.

Jim indicated that prior to running CAMx with an ERF adjustment, ISC will be re-run with the adjustment applied as an area-wide constant multiplier and separately with the adjustment applied on a grid cell basis to see which provides a better reconciliation (i.e., Goodness-of-Fit Test) with the ambient measured HRVOC concentrations. Additionally Jim indicated that when the 2006 STARS point source data is available, the ISC and PSCF Type 2 analyses will be conducted to develop ERFs for 2006.

Questions and comments that arose during Jim's presentation included:

- Whether the number of back trajectory points tallied within a grid for high concentrations versus low concentrations is biased, since high concentrations are typically associated with lower wind speeds, which could increase the number of points within a grid;
- Why the median, rather than the mean value was selected;
- Why has the focus of the ERFs been on the point sources;
- Has there been any consideration to using the decay scheme in ISC to account for the chemical reactivity;
- Has there been any consideration of applying this procedure to HAPs, such as benzene; and
- Has there been any consideration of using inverse modeling w/DDM to develop ERFs.

Jim acknowledged that there may be unanticipated biases in the approach, which may be accentuated by the constraint imposed by the use of only "straight-line" winds. Jim explained that the median was selected because the distribution of tallied concentrations within a grid is generally skewed and so the median is a better metric. With regard to the focus on point sources, Jim explained that the ISC modeling analysis did include area and mobile source emissions. So far the ERFs have only been applied to point sources, but applying the ERFs to all sources will be investigated. There was a fair amount of discussion during Jim's presentation about using the decay scheme in ISC to account for the chemical reactivity. Jim acknowledged that by not accounting for chemistry (i.e., no decay scheme in ISC), the ERFs are smaller, especially for the very reactive compounds, such as propylene. Jim indicated that similar to the application for butanes, this procedure could be applied to benzene. Jim acknowledged that there are

other procedures, such as reverse modeling that could be applied to reconciling the emissions and TCEQ would consider them as needed.

8-Hour Coalition Update – Al Hendler, URS

Al's presentation, entitled, "HGB Ozone Trends," addressed the effects mild temperatures and wet weather had on ozone concentrations during 2006 and 2007, especially the daily maximum 8-hour ozone concentrations. (Note: Al's presentation is available on the SETPMTC web-site: http://www.tceq.state.tx.us/implementation/air/airmod/committee/pmtc_set.html).

Al explained that the approach uses the Classification And Regression Tree (CART) analysis with primarily meteorological parameters to define an "ozone conducive day (OCD)." Then the ratio of the number of OCDs with daily maximum 8-hour ozone concentrations > 84ppb to the total number of OCDs is determined for each year for the HRM sites. This ratio is used for the trend analysis, since it should remove the influence weather related parameters (e.g., temperature, rain) have on the daily maximum 8-hour ozone concentrations.

Al presented a graphical display of the CART analysis, which showed the OCD to be defined principally by the average (0800-1600 hours) wind speed (i.e., ws < 6.4 mph), the maximum daily temperature (i.e., max.temp > 74.3 degrees) and the daily temperature range (i.e., [max – min] > 13.4 degrees). Al then presented a graphical display of the trend analysis from 1990 through September 2007, which indicates a decrease in the ratio, with 2007 having an especially low ratio. Al also discussed noteworthy caveats concerning the trend analysis, including the "broad" definition, as per CART, that results in a large number of OCDs that have notably low daily maximum 8-hour ozone concentrations, the lack of rain or cloudiness in the CART analysis, and that only the seven HRM sites were used.

Al presented additional graphical displays showing the reduction in reported NO_X emissions for point sources in the HGB area (i.e., ~70%; 1996 to 2005); and the reduction in monitored ambient HRVOC concentrations at long-term monitors (i.e., ~50%; 1997 to 2007).

Al summarized his presentation saying that even with the noteworthy caveats to the trend analysis, the lower number of 8-hour exceedance days (i.e., ~50% of monitors had 2007, 8-hour ozone design values $\leq$ 84ppb), as well as the lower number of 1-hour exceedance days (i.e., in 2007, 40 of 44 monitors had $\leq$ 1 exceedance of the previous 1-hour NAAQS) may be related more to the emission reductions than the weather conditions in 2007.

The major comment during Al's presentation was the lack of any appreciable significance to 8-hour ozone from rain and/or cloudiness in the CART analysis, which seems counter-intuitive. Al indicated that solar radiation (to represent clouds) and rain > 0.01" were included in the CART analysis.

Adjourn

The meeting adjourned with a brief discussion of the scheduling of subsequent meetings in 2008. Dick suggested that the meetings continue to be scheduled bi-monthly, starting in February 2008. Jim suggested that for meetings spanning the lunch hour (e.g., 10am to 3pm), we consider have lunch delivered, so as to avoid eating late lunches. There was general agreement to these suggestions. Graciela indicated she would look into scheduling the conference room, and Dick would give her a list of dates.