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**HARC Project H12/HRB Final Report**

**Role of Modeling Assumptions in the Houston Mid-Course Review**

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## PROJECT SUMMARY

TCEQ has developed completely new ozone modeling databases for use in the current Houston-Galveston area (HGA) Mid Course Review of the State Implementation Plan (SIP) for ozone with concentrations averaged over 1-hour. This modeling reflects major new insights into the ozone problem in the HGA that emerged from the TexAQS 2000 field study. The technical foundation of new SIP modeling has been comprehensively updated and improved from the previous 1993 ozone modeling, with improvements to emission inventories, meteorological modeling and air quality modeling developed by the TCEQ staff and numerous contractors. The new modeling databases have now been applied in the proposed Mid Course Review SIP and it is an appropriate time to investigate, for the 1-hour ozone attainment, issues such as uncertainty, robustness, and relationships to new 8-hour emerging requirements.

This report summarizes research findings of the University of Houston on the multi institutional project, "Role of Modeling Assumptions in the Houston Mid-Course Review." The main effort of the UH is to modify emissions inventory for different land use land cover data and to run various sensitivity analyses using some CAMx and some CMAQ runs.

This project intended to answer the following two questions:

- Do the input and operational assumptions used in the proposed SIP modeling introduce bias into predicted 2007 ozone concentrations?  
The assumptions that will be considered in this work include the biogenic emission estimates, land cover characterizations, imputed inventory of (Highly Reactive VOCs) HRVOCs and chemical mechanism details.
- Do any potential biases in model predicted 2007 ozone concentrations impact the effectiveness of proposed control strategies?

This project was a joint effort between the University of Texas, the University of North Carolina, the University of Houston, and ENVIRON Corporation. Although all four of the institutions have been involved in all of the tasks, we summarize the specific research findings of the University of Houston to assess the impact of land covers and choice of mechanism on model performance.

University of Houston performed several sensitivity simulations with CAMx and CMAQ to characterize uncertainties originated from model inputs and science algorithms used. Six different variations of biogenic and anthropogenic emissions inputs were used for the CAMx and CMAQ simulations of Houston-Galveston area at 4-km resolution for the simulation period of August 23 ~ August 31, 2000.

We compared CAMx and CMAQ results to see if the two models produce similar ozone concentration differences when different LULC data are used. Except for the unusual peaks in late afternoons and nighttime on August 23, 24, and 30, CMAQ predicts around 30% lower isoprene concentrations at the Clinton site due to its higher eddy diffusivity values used with the TCEQ-LULC data. When we used the TFS-LULC data for biogenic estimation and dry deposition, both models show decreased isoprene concentrations, especially on August 30 and 31. Compared to the Clinton site, isoprene concentrations at La Porte were relatively low and both models overestimated the ambient concentrations by a factor of 2~5.

Given emissions and meteorological data, the models behaved similarly and matched well with ozone observations except at some high peaks. CAMx showed higher values corresponding to the observed peaks; while CMAQ compared better than CAMx with measurements in the low to medium ozone concentration range, say 60 -100 ppb. CAMx simulation with TCEQ-LULC data presented a high correlation with the observations and CAMx with TFS-LULC showed slight underestimations. CMAQ simulations were insensitive to the changes in the LULC data

When compared with NOAA aircraft data, CO showed much larger discrepancies between two models than other species observed at high altitudes, indicating that the mixing characteristics of the two models are significantly different. CO is a relatively inert species and is not affected by the chemistry of the rapid ozone production chemistry. Also, a large portion of the CO emission is originated from the mobile sources. Therefore, it can be considered as a trace species that helps to explain the mixing properties of air quality models. CAMx over-predicted CO concentrations compared to the observations and CMAQ. The total reactive nitrogen species (NO<sub>y</sub>) showed similar behavior as CO. With CMAQ we performed an additional sensitivity test with the CMAQ and CAMx eddy diffusivity algorithms. These analyses provided some indication that mixing was better represented in CMAQ than CAMx.

Because the imputed emissions inventory included large amount of additional HRVOC emissions such as OLE and ETH, the surface concentrations of these species showed high overestimations, especially during nighttime. Although a large amount of OLE and ETH emissions were added as low-level emissions in the imputed emissions inventory (over the regular inventory by a factor of 7 ~ 13), the model simulations still showed serious under prediction of the HRVOC concentrations compared to the canister measurements in upper layers. On the other hand, the surface concentrations were extremely over predicted in both CAMx and CMAQ models. We suspect that the additional HRVOC required to increase ozone reactivity in the HGA must come from stacks and flares with effective release heights above the lowest model layer, and not mostly from low-level emissions, as is effectively assumed in the SIP model. In this regard, we found that doubling or quadrupling exhaust velocities and increasing default heights of HRVOC emissions were not sufficient to raise most emissions beyond the lowest model layer. As a result, there remained a high bias at the surface and a low bias aloft in simulated HRVOC concentrations as compared to observations. Simulations with the regular (i.e., without the additional HRVOC) anthropogenic emissions showed better agreement with the surface HRVOC measurements at low concentration range, but misses intermittent high concentration events. Without the additional HRVOC emissions, simulated surface O<sub>3</sub> concentrations were much lower than the imputed case. CAMx showed larger sensitivity of the O<sub>3</sub> concentrations to such emissions changes than CMAQ. With the regular inventory, CAMx and CMAQ's ozone predictions were very close to each other.

It is important to check if we can effectively reduce ozone for the HGA 8-county non-attainment area in the future years through the emissions controls prescribed in the SIP. CAMx and CMAQ were utilized to simulate future conditions using the TCEQ-prepared future emissions ('fy07j cs03 harCap'), coupled with biogenic emissions estimated with the TCEQ-LULC and TFS-LULC data. Similar to the base case simulations, CAMx predicts higher ozone concentrations than CMAQ except for August 23<sup>rd</sup>, 2000. However, for some days, CAMx showed higher maximum ozone concentrations with TFS-LULC than with TCEQ-LULC. Especially, the ozone concentrations

predicted with TFS-LULC for August 25<sup>th</sup> does not satisfy the 1-hour standard (125 ppb), while the concentrations simulated with TCEQ-LULC is lower than the standard. On August 30<sup>th</sup>, all four simulations show that the maximum ozone concentrations for the area exceed the 1-hour standard value.

Even with the imputed HRVOC emissions, it was difficult to predict high ozone peaks in the vicinity and downwind of the Ship Channel and other highly VOC rich areas. Downtown Houston is NO<sub>x</sub> rich because of on-road and non-road mobile sources and the lack of large direct VOC sources. The VOC/NO<sub>x</sub> ratios in the area are quite lower than those for the Ship Channel area where lots of VOC emissions come out of the petrochemical plants. We believe the low ozone reactivity downwind of the Ship Channel is due to the lack of radical sources. One of direct radical sources for the ozone chemistry is the photo-dissociation of NO<sub>2</sub> molecules by sunlight. Therefore, we performed a sensitivity study modifying the implicit splitting ratio of 90% to 10% between NO to NO<sub>2</sub> ratio in the NO<sub>x</sub> emissions in the emissions processing to understand the impact of free oxygen atoms on the O<sub>3</sub> production around the downtown area, in which no major VOC sources are identified. When the NO<sub>2</sub> splitting ratio is increased to 20%, the predicted ozone increased 10-16 ppb depending on the simulation dates. This sensitivity test are made with an assumption that more NO<sub>2</sub> (instead of NO) becomes available from the high NO<sub>x</sub> emissions area to compensate the shortage of the ozone forming reactivity caused by NO emissions. As such, it does not answer what process is responsible for the lack of reactivity and therefore does not tell us how to make up for that. However it is suggested that more HRVOC concentrations or less NO<sub>x</sub> concentrations in the downtown area, either through reduction of local NO<sub>x</sub> emissions or downwind transport of the enhanced VOC emissions from Ship Channel area, can introduce higher simulated ozone concentrations, thus reducing the under-prediction of peak concentrations.

More intense solar radiation can also provide additional radical sources in the photochemical system. The solar radiation intensity is one of the meteorological factors that determine the rates of photolysis and chemical reactions in the atmosphere. Since the cloud cover affects the availability of solar radiation, it becomes important to correctly estimate the cloud amount. To estimate the O<sub>3</sub> concentrations under the maximum solar radiation conditions, we performed sensitivity tests with and without cloud. The CMAQ simulation result showed that the maximum O<sub>3</sub> concentrations increased by 10 ppb for August 30, 2000 at 15 CST and the difference were spatially as high as 40 ppb of O<sub>3</sub> concentration over downtown Houston and downwind area. O<sub>3</sub> concentrations in the middle of boundary layer increased up to 20 ppb with no cloud simulations.

Finally, we have studied effects of using different chemical mechanisms on the ozone simulations. Because of the various technical issues of representing explicit chemical species with the current Texas emissions inventory (EI), the scope of this research was limited in such a way that we used the older EI, Base4a, and performed simulations with SAPRC only with CMAQ. The SAPRC mechanism produced higher ozone concentrations than CB-4 while most of the precursor species concentrations look very similar to each other. Further study with the new emissions inventory will be needed to confirm this finding.

In conclusion, we believe that once the uncertainties in the input data are reduced, and when appropriate transport and chemical algorithms are used, models can adequately simulate the

observed ozone events and we can use them to demonstrate effects of emissions control strategies. The most important modeling improvements that are needed include adjustments to the following:

- Vertical diffusivity formulation
- PBL and land surface physics and/or data assimilation schemes affecting model horizontal winds
- HRVOC event emissions and stack parameters for stack and flare emissions
- Urban radical sources downwind of the Houston Ship Channel
- Cloud cover and photolysis rates
- Chemical mechanism speciation and reaction schemes.