Executive Summary

for the Texas Environmental Research Consortium Project H12-8HRB

"Impact and role of air quality modeling assumptions in the development of revisions to the Houston State Implementation Plan for attaining the ozone air quality standard "

Submitted by
David Allen*, Elena McDonald-Buller, Yosuke Kimura, William Vizuete, Linlin Wang and Alba Webb
Center for Energy and Environmental Resources
University of Texas at Austin

Greg Yarwood, Sue Kemball-Cook, Chris Emery
ENVIRON International Corporation

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The Texas Commission on Environmental Quality (TCEQ) has devoted considerable resources to enhancing regulatory modeling, emission inventories and analytical tools that are used in evaluating the State Implementation Plan (SIP) for attaining the National Ambient Air Quality Standard for ozone in the Houston-Galveston area. The advances that have been made incorporate new insights into ozone formation and accumulation in the Houston-Galveston area that emerged from the Texas Air Quality Study (TexAQS). Major improvements continue to be made in emission inventories and meteorological modeling. Nevertheless, some uncertainties still remain. The goals of the project summarized in this document were:

- To determine whether input and operational assumptions used in the SIP modeling introduce bias into predicted ozone concentrations, and
- To determine whether model biases might impact the predicted effectiveness of proposed control strategies.

Specifically, model assumptions and uncertainties that were examined included the effects of fires, uncertainties in biogenic emissions, uncertainties in meteorological model predictions, grid resolution, the choice of chemical mechanism, and imputed inventories of highly reactive volatile organic compounds (HRVOCs) and other volatile organic compounds (OVOCs). The project was a joint effort between the University of Texas, the University of North Carolina, the University of Houston, and ENVIRON Corporation. This Executive Summary and supporting documentation describes the work done by the University of Texas and ENVIRON on (1) the impacts of fires, (2) uncertainties in biogenic emissions, (3) uncertainties associated with the choice of chemical mechanism, and (4) modeling fine spatial scale ozone features observed in Houston. For each of these topics, the nature of the uncertainty, an assessment of the potential biases, and recommendations for addressing the uncertainty in future modeling are described. Additional details are available in supporting documents.

*Author to whom correspondence should be addressed: allen@che.utexas.edu; tel: 512-475-7842

Impact of Fires

Issue: Extensive wildfires occurred during the summer of 2000 in southeast Texas. The air quality impacts of these wildfires were included in air quality modeling of photochemical episodes that occurred during the summer of 2000 and in the emission inventories used in the attainment demonstration. However, it is unlikely that wildfires this extensive will occur in all future years. Therefore, in demonstrating attainment for the national ambient air quality standard for ozone, a reduced level of fire activity, compared to the fire activity in 2000, should be assumed in future years.

Key Findings: The peak ozone concentrations predicted for future years were evaluated using the assumption of no fires and the assumption that wildfires would occur at the same level as in 2000. While fires did have significant (>30 ppb) localized impacts on ozone concentrations, assuming fires were as intense as in 2000 added only about 1 ppb to area-wide peak ozone concentrations in the attainment demonstration.

Recommendations: In the 2000 modeling episode, large fires were not directly upwind of areas where area-wide peak ozone concentrations were observed. This fortunate circumstance may not continue in future years. It would be useful to establish an on-going mechanism, using satellite data, to track fire locations and magnitudes so that if natural fires have significant impacts on peak ozone concentrations in future years, the magnitude of the impact can be documented.

Uncertainties in Biogenic Emissions

Issue: The largest source of reactive hydrocarbon emissions in southeast Texas is vegetation. Biogenic emissions, particularly from certain species of trees, will continue to dominate the hydrocarbon portion of the emission inventory in future years; the presence of trees also affects the rate at which pollutants are removed from the atmosphere and the temperature of the land surface, as well as other meteorological parameters. The ever-changing land use patterns in the Houston area change tree cover and present challenges in modeling biogenic emissions and atmospheric processes controlled by land cover. The attainment demonstration modeling uses landcovers that were current in the 1990s; these landcovers have undoubtedly changed and will continue to change.

Key Findings: The sensitivity of air quality model predictions to land covers was evaluated using a variety of fully and partially developed land use assessments. The effect of landcovers on both biogenic emissions and deposition was assessed, and the analyses indicate that uncertainties in biogenic emissions, associated with variations in tree speciation in the landcover data, introduced much greater uncertainties in predicted ozone concentrations than uncertainties in deposition associated with variations in land cover assignments. While the differences between predicted ozone concentrations, based on different land cover data, can be significant, the characterizations of land covers used in the current photochemical modeling are the best comprehensive data available. It is not possible, with current information, to assess whether the existing landcovers bias air quality model performance. However, in the course of comparing predicted and observed isoprene concentrations, it was discovered that the current SIP model over-predicts isoprene concentrations, compared to observations, by a factor of 2-5 at multiple ground sites for all of the landcover assignments. This over-prediction decreases as vertical diffusivity is increased in the model. Increasing vertical diffusivity decreases ground level concentrations of all ozone precursor species, but has a complex impact on ground-level ozone concentrations due to spatial variations in VOC/NO_x ratios.

Recommendations: Sensitivity analyses suggest that some projected changes in land covers have the potential to significantly reduce air pollutant concentrations, while other projected changes might significantly increase concentrations. To track these changes, it would be useful to regularly update landcover data, using a combination of satellite data assimilation and ground surveys, including tree species counts. In addition, comparisons between observed and predicted ground-level isoprene concentrations suggested that model predictions are sensitive to changes in vertical diffusivity parameters; measurements that characterize vertical diffusivity should be undertaken in future air quality field campaigns.

Uncertainties due to Choice of Chemical Mechanism

Issue: Models of atmospheric processes use simplified photochemical reaction mechanisms. These simplified photochemical mechanisms condense the large number of atmospheric species into a smaller number of "lumped" chemical species; the mechanisms also typically collapse rapid, multi-step chemical processes into single reactions. The two mechanisms that are most commonly used in air quality models are the [California] Statewide Air Pollution Research Center (SAPRC) mechanism and the Carbon Bond (CB) mechanism. Both mechanisms are approved for use by the U.S. EPA and are updated periodically to correct deficiencies or to incorporate new experimental findings. The versions of the mechanisms currently in use are SAPRC99 and the "OTAG version" of CB-IV from 1996. The State of Texas used the 1996 CB-IV mechanism in its attainment demonstration. A more recent version of CB-IV called CB2002 was used for sensitivity tests. Sensitivity tests also considered the importance of NOx recycling reactions that are omitted from all versions of CB-IV.

For most urban areas, all versions of CB-IV and SAPRC mechanisms yield similar results, but for the modeling done of the summer of 2000 in southeast Texas, the SAPRC mechanism leads to concentrations of ozone that are 30-50 ppb higher than in all versions of CB-IV. Because of uncertainties in the emission inventories for the Houston-Galveston area, it is not clear which of the two mechanisms is more accurate, and it was not clear whether the emission control package proposed for Houston would lead to predictions of attainment with both of the mechanisms.

Key Findings: The CB2002 version and OTAG versions of CB-IV produce similar ozone levels and similar responses to added HRVOC emissions. Including NOx recycling reactions in CB-IV increases ozone transport into the Houston area by several ppb. The comparisons between SAPRC and all versions of CB-IV demonstrated that although the two mechanisms lead to very different predictions of ozone formation under the conditions modeled for the summer of 2000, once the proposed control strategies are applied, the predictions converge. This means that both SAPRC and CB-IV (all versions) predict similar absolute ozone concentrations after controls are applied. Reducing predicted ozone concentrations to a target absolute level is how attainment is demonstrated for the NAAQS for ozone, with concentrations averaged over 1-hour. However, when demonstrating attainment with the NAAQS for ozone with concentrations averaged over 8 hours, relative reductions in ozone predicted by the model are used. SAPRC predicts consistently larger relative reductions in ozone, for the current set of controls in Houston, than CB-IV. In particular, SAPRC is more sensitive to NOx emission reductions than CB-IV. The magnitude of the difference varies from day to day.

Recommendations: Because of the significant differences in relative ozone reductions predicted by SAPRC and CB-IV for Houston, the causes of the differences should be identified, and a mechanism appropriate for Houston conditions should be selected. This mechanism selection will be particularly important in developing air quality plans for meeting the NAAQS for ozone with concentrations averaged over 8 hours. Evaluating and selecting mechanisms will require a new generation of air quality field data. Plans to collect those data are a part of the second Texas Air Quality Study (TexAQS II)

High Resolution Grids

Issue: Ambient monitoring in Houston during TexAQS 2000 and other studies revealed localized high ozone levels resulting from HRVOC releases. Photochemical modeling is better able to replicate these fine scale features using a 1-km grid than a 4-km grid. Meteorological data were developed at 4-km resolution and interpolated to 1-km for ozone modeling. Ozone modelers have little experience modeling ozone at 1-km resolution and the Houston modeling is breaking new ground. The dispersion of point source emissions in very high resolution grids was investigated to provide guidance on strengths and limitations to fine spatial scale modeling.

Key Findings: Point source plume dispersion in a very high resolution grid (200 m) was evaluated against results from a Lagrangian puff model embedded within a 4-km grid. The advantage of a puff model over a grid model is that the puff model can better represent how dispersion changes at fine scales as the plume grows in size. The puff model showed slower dispersion than the grid model at very fine plume scales (few hundred meters wide) because the grid was unable to resolve the plume (excess artificial diffusion on the grid). The puff model showed faster dispersion than the grid model when the plume spanned the intermediate scale from a few hundred meters to 4 km because the process of interpolating winds from 4 km to 200 m misses important dispersion characteristics at the intermediate spatial and temporal scales. It was also found that high vertical resolution can increase predicted ground-level ozone concentrations.

Recommendations: High-resolution grids using interpolated meteorological data may capture some features at the expense of others. For Houston, a 1 km grid driven with 4 km meteorology can capture rapid ozone formation near HRVOC releases but underestimates the dispersion of larger scale ozone features such as the urban plume. Additional research is needed to develop and test modeling procedures that address both needs. Potential approaches include: (1) high spatial and temporal resolution meteorological fields; (2) modeling HRVOC releases using plume-in-grid modeling approaches; (3) adding additional diffusion to high resolution grids when they are driven by interpolated meteorological data.

Synthesis of findings

As the result of this project, four major issues have been identified which have the potential to cause biases in modeling results:

- Future ozone concentrations are biased high by assuming that fires occur at the higher than normal intensity that occurred in 2000;
- Both increases and decreases in ground-level ozone concentrations would occur if vertical diffusivity parameters were increased in the model. Increases would occur in areas where NO titrates ozone at ground level; decreases would occur in regions that are not rich in NO. While model predictions are sensitive to vertical diffusivity, only indirect evidence on values of diffusivity parameters are currently available;
- Relative ozone reduction factors for control strategies are more responsive to NOx reductions with one commonly used chemical mechanism than with the other commonly used mechanism; and
- Model predictions of ozone concentrations are sensitive to the horizontal and vertical resolution used in the model, especially in areas with high densities of point source emissions. Predicted ozone concentrations generally increase as horizontal and vertical resolution is increased, however, the validity of current meteorological models at fine scale (<4 km) horizontal resolution introduces poorly understood uncertainties into the air quality modeling.

Uncertainties in biogenic emissions, which were also considered in this work, did not by themselves introduce a quantifiable bias into the modeling. The impacts on control strategies of alternate approaches to modeling fine scale ozone features have not been investigated at this time.

The potential biases documented in this work must be balanced against other biases that will be reported on in other reports. These include the impact of episodic releases of reactive hydrocarbons from industrial sources and potential uncertainties in industrial emission inventories.