

EXECUTIVE SUMMARY

This report summarizes the model sensitivity study results of the baseline CAMx simulations utilized for the East Texas Source Apportionment Study (ET-SAS). The prime objective of the ET-SAS was to evaluate the sensitivities of O₃ to “other” (non-highly-reactive) VOC (OVOC) emissions from the Ship Channel area. The ET-SAS modeling work was performed by the Atmospheric and Environmental Research, Inc (AER) utilizing the Comprehensive Air Quality Model with extensions (CAMx) model with the Direct Decoupled Method (DDM) to calculate sensitivity coefficients.

To provide the model input data, as well as baseline air quality simulation results to AER, the University of Houston (UH) performed meteorological data preparation, emissions processing, and CAMx air quality modeling for the August 22-31, 2000 TexAQS episode. The MM5 meteorological modeling data was prepared by Texas A&M University (TAMU). For the State Implementation Plan (SIP) modeling, the Texas Commission for Environmental Quality (TCEQ) usually utilizes the CAMx model with the Carbon Bond Version 4 (CB-4) mechanism. However, to study the sensitivity of the Houston-Galveston-Brazoria (HGB) area ozone to the OVOC emissions, the CAMx model with the SAPRC mechanism was deployed in this project.

This study represents UH’s most recent effort to generate the emissions input for SAPRC99 mechanisms for CAMx and CMAQ using the EPA’s SMOKE system. The current emissions input for CAMx for the SIP modeling was processed by TCEQ utilizing the EPS system. To evaluate the differences in the internal speciation data and other characteristics of the SMOKE processing from EPS-3, we compared the CAMx simulations with two differently obtained emissions for the CB-4 mechanism. To establish the baseline CAMx simulation results for the OVOC sensitivity study, various model sensitivity studies were performed and the findings are summarized below.

Findings

CAMx simulations with EPS and SMOKE-processed emissions presented comparable overall spatial distributions of predicted concentrations, but the CAMx with SMOKE data resulted in lower maximum ozone concentrations than with EPS-3 for the CB-4 mechanism.

The differences in O₃ concentrations predicted with the two CAMx horizontal advection schemes, PPM and Bott, were below 10 ppb most of the time and usually less than 5 ppb. In general, Bott showed higher peak ozone concentrations.

CAMx and CMAQ simulations with SAPRC99 always showed higher daily maximum 1-hour O₃ concentrations than those with CB-4 for the same simulations, but tended to over-predict ozone at concentrations below 120 ppb.

A key indicator of chemical mechanism behavior is the tendency for CB-4 to underestimate PAN and overestimate HNO₃ concentrations compared to SAPRC99. CB-4 may therefore not be locally recycling NO_x as much as observations indicate, possibly depressing ozone production.

CMAQ showed greater sensitivity to the use of different mechanisms than CAMx. Compared to CAMx version 4.03, CAMx version 4.20 predicted higher surface O₃ concentrations, sometimes over 30 ppb for the episode. The difference was largest- on August 25, followed by August 30 and August 26, 2000.

A sensitivity study of the OVOC imputed emissions were conducted with CMAQ. Compared to CMAQ with HRVOC imputation only, CMAQ simulation with 3.8 times additional OVOC emissions predicted higher daily maximum 1-hour O₃ concentrations by up to 5 ppb except on August 25, 2000, when the increase in O₃ concentrations was as high as 20 ppb. This maximum response to OVOC is consistent with AER's computed DDM maximum sensitivity in downtown Houston of 4 ppb per 100% change in OVOC Ship Channel emissions.