1 Executive Summary

The purpose of this project is to demonstrate the use of adjoint sensitivity analysis and data assimilation techniques on air quality problems in Texas. This exploratory research is not intended to directly address operational issues on a regulatory timetable, but to evaluate methods already in use within the atmospheric science community for possible application to SIP modeling in the future. In this framework it was not deemed necessary to use an operational grid typical of SIP ozone attainment studies; the simulations have been carried out using the STEM model(Sulphur Transport Eulerian Model) on relatively coarse grids (36Km) for a proof-of-concept demonstration. Future studies should perform sensitivity analysis and data assimilation at operational resolutions.

The second part of the report focuses on two episodes in June 2005. During June 19 the main flow direction which influences the DFW area is from the East. During June 23 the main flow direction influencing the DFW area is from the South. The main findings of this project are summarized below.

1.1 Adjoint sensitivity analysis

Direct decoupled sensitivity analysis is a source-oriented approach: the perturbation at the source is propagated forward in time through the computational domain. Adjoint sensitivity analysis is a receptor-oriented approach: the sensitivities of a cost function (e.g., the concentration of a certain species at a receptor location at a certain time) with respect to earlier perturbations at all gridpoints is computed effectively.

We demonstrate the use of adjoint sensitivity analysis for a receptor that is located at the ground level on the DFW area. Simulations are carried out using STEM model with a resolution of 36Km. We run simulations for two 28-hour intervals in June 2005 (from 8pm CST June 18 to 0am CST June 20 and from 8pm CST June 22 to 0am CST June 24). One set of simulations focuses on a passive tracer, and illustrates the influence of the meteorological conditions. The other results show the areas where changes in precursors (O_3, NO_2, and HCHO) have the maximal impact on the DFW ground level ozone.

1.2 Data assimilation for the reanalysis of chemical fields

Data assimilation is the process by which measurements are used to constrain the model predictions; the information from measurements can be used to obtain better initial conditions, better boundary conditions, enhanced emission estimates, etc.

When the initial conditions of the model are adjusted to better fit observations we perform a rigorous re-analysis of chemical fields which leads to distributions of tracers that are consistent with both the observations and the model.

We performed data assimilation for the initial conditions for two 24-hour episodes (starting at 0am CST on June 19 and on June 23 respectively). Data assimilation uses the AirNow ground level observations for stations above Texas. The re-analyzed chemical fields show a considerable improved agreement with the AirNow observations (the R^2 correlation coefficients increase from 0.4-0.5 to over 0.7).

1.3 Conclusions

Adjoint sensitivity analysis and data assimilation have an excellent potential to complement other approaches in Texas air quality studies. Adjoint sensitivity analysis allows us to assess the areas that have the largest impact on a given receptor site. Data assimilation allows us to combine the information from both observations and models, and to obtain best estimates (in a statistical sense) of the three-dimensional distribution of tracers. Reanalyzed chemical fields are important to better understand past episodes. Reanalyzed fields can be used to initialize air quality forecast runs and have the potential to improve air quality predictions.

Our research has been based on coarse-resolution runs of the STEM model for a variety of meteorological episodes in the years 2004 and 2005, as described in both Parts I and II of this report. Together, these episodes show transport towards the Dallas-Ft. Worth (DFW) area from all cardinal directions of East, West, North, and South, as portrayed by estimated back trajectories. A caveat is that Texas emissions inputs assumed for 2004 (NEI99) and 2005 (Byun et al., 2006) are very different. Policy implications stemming from our work in both Parts I and II are as follows:

- The Gulf Coast has the potential to strongly influence ozone exceedances in the Dallas-Ft. Worth (DFW) non-attainment area through long-range transport, depending on the meteorological episode.

- Long-range transport of formaldehyde, especially from the Gulf Coast, may rival long-range transport of NOx and ozone in its impact on DFW surface ozone. The actual magnitude of impact is very dependent on both the strength of southerly flow and emissions inventory assumptions.

Vertical mixing of ozone and precursors from the upper Planetary Boundary Layer (i.e., about 1.5 km above ground) may be an important influence on DFW ozone. This would require more attention to State Implementation Plan (SIP) model performance in layers aloft, and not just at the surface.