Planning and Execution of the NE Texas Plume Study (NETPS) and LESchem for Plume Studies

FINAL REPORT

Tasks 4 and 5 of TERC Project H44

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EXECUTIVE SUMMARY

TERC Project H44 was entitled "Modeling Activities at UAH in Support of TexAQS II", and was comprised of five Tasks, of which Tasks 1-3 were under the direction of Co-PI Dr. Richard McNider and Tasks 4 and 5 were under the direction of Co-PI Dr. Noor Gillani. This is the Final Report of Tasks 4 and 5. Task 4 was under the general title "Large Eddy Simulation with Chemistry for Characterization of Industrial Plumes"; Task 5 was under the general title "NE Texas Plume Study (NETPS)", but was more specifically aimed at development of detailed planning for the field measurement program of NETPS and at the execution of the field study in NE Texas during August 2005, the last month of the project period of H44.

The work of Task 4 followed earlier work related to preliminary application of the UAH-LESchem Model (Large Eddy Simulation with Chemistry) under TERC Projects H6B and H26. LESchem was developed in an EPA project during 2001-02 and there applied to simulate near-source power plant plume chemistry. It was applied in H6B to the Sweeny petrochemical plant plume in which ozone precursors VOC and NOx are nearly co-emitted and, on a summer day, undergo rapid initial (near-source) chemistry. That was the first realistic application of an LESchem model to a petrochemical source plume and yielded quite realistic simulation of the aircraft observations of plume chemistry in the isolated Sweeny plume of 28 August 2000 in the Houston-Galveston area. It was shown that eddy-scale effects are most pronounced in the first hour or so of petrochemical plume chemistry. In H6, the UAH-LRPM was also applied in top-down emissions verification mode, not only to isolated petrochemical plumes like Sweeny, but also to the multi-source ship channel megaplume. LESchem could not be applied to the ship channel plumes complex because of computational constraints related to the fact that the computer code of the embedded chemistry module of it (developed in-house at UAH) was not parallelized as the original physics code (RAMS-LES) was. Thus, a major objective of Task 4 of H44 was to parallelize the LESchem code fully, then apply it to the ship channel complex (requiring a simulation domain of at least 50km x 30 km horizontally, a domain size greater than any previously attempted in LES simulations by at least an order of magnitude). It was the objective ultimately to perform a study aimed at development of parameterizations of the eddy-scale chemistry (based on LESchem applications) for application in LRPM. The parallelization of LESchem turned out to be of a much greater scope than anticipated and took up much of the project period. However, we did complete and test it successfully for the Sweeny plume. We also found the task of generating realistic initial and boundary conditions for the large ship channel domain within an urban environment to be non-trivial. At the end of the project, we were in this stage of the work. The work is thus unfinished and will need further effort to complete testing of it for the ship channel complex and to develop the parameterizations.

The work of Task 5 (NETPS) involved mainly the field study planning, and finally, in the last month of the project period, participation in the execution of the field study. The motivation for the study was based on past surface ozone observations in the DFW ozone non-attainment area, which had indicated that upwind inflow into the DFW area contributed nearly 2/3 of the peak ozone observed in the non-attainment area on high ozone days. Hence, the main objective of the field study was to perform 3-D aircraft sampling in large point-source plumes from upwind point sources (mainly power plants) upto 250km upwind of DFW, in order to quantify the ozone impact of these plumes on high ozone days. The planning was performed very thoroughly based

on study of the sources in the region, the meteorological climatology, and the anticipated transport-chemistry scenarios. A detailed Experimental Plan document was developed and circulated to the study participants well ahead of the field study period, which was set at the month of August 2005 based on expected optimum measurement conditions. The most likely upwind direction was identified as the SE quadrant, and the target sources were those upto 250km upwind of DFW. Three sets of target sources were identified: those in Zone A including the DFW area and areas immediately upwind, mainly Ellis CO (the Zone A impact was designated by TCEQ as priority 1 of NETPS); those in Zone B to the S and SE of DFW at distances ranging between 100 and 250 km (designated as priority 2); and finally, sources in the Tyler-Longview area about 200-250 km to the east of DFW (designated as priority 3). Partners in the study were TCEQ (surface monitoring, some met measurements, funding of the aircraft measurements by TVA, and guidance related to the desired objectives), HARC (funding for UAH, TAMU, and UH, and certain logistical support), TVA (aircraft measurements), TAMU (certain met measurements and met forecasting, and deployment of the PTRMS in the aircraft), UH (regional chemistry forecasting), and UAH (lead science team for study planning and direction --- Gillani team, and plume transport forecasting based on Lagrangian particle modeling --- McNider team).

The Midway Regional Airport near the town of Waxahachie in Ellis CO was chosen as the base airport for the aircraft flights, and an Operations Center was set up in the Civic Center of Waxahachie. Daily weather forecast and planning meetings were held there, and post-mission data review meetings were held as necessary and possible. The field study was significantly marred by very unusual and unfavorable meteorological and chemical ambient conditions during much of the month: the Eastern USA regional background, as well as the local background, were unusually clean for August for a good part of the month; meteorological conditions, too, were quite unlike the local climatology, with wind directions which failed to bring the anticipated distant plumes (Zone B, C) into the DFW area, as well as an early stagnant period giving way to an extended period with very strong winds, ending finally with strong northerly flow related to hurricane Katrina. The best measurement conditions were encountered between August 18 and 26, during which period 5 aircraft missions were performed (3 ½ for Zone A sources and 2 ½ for Zone B sources --- one mission was a combined Zone A/Zone B mission); an Ellis CO sources mission was performed under clean conditions on August 11, and two more Zone A missions were performed on August 28 and 30 under Katrina-related northerly flow, and a final Zone A mission was performed on the last day of the study (Aug 31) under relatively stagnant conditions. Overall, 9 missions were performed compared to the seven planned, and a rather solid dataset has been generated for the Zone A scenarios, with 2 ½ missions also of Zone B sources under less than ideal conditions. No Zone C missions were performed as those plumes failed to come into DFW during the study period. Thus, we believe that reasonably good, if less than ideal, data exist for the priority 1 and 2 objectives.