EXECUTIVE SUMMARY

Problem Statement

The purpose of this project is to advance our understanding of Texas Air Quality (AQ) by utilizing satellite observations and the new advances in biogenic emissions modeling to improve biogenic emission estimates used in Texas State Implementation Plan (SIP) modeling activities.

One of the challenges in understanding Texas air quality has been the uncertainties in estimating the biogenic hydrocarbon emissions. Biogenic volatile organic compounds (BVOCs) play a critical role in atmospheric chemistry, particularly in ozone and particulate matter (PM) formation. In southeast Texas, BVOCs (mostly as isoprene) are the dominant summertime source of reactive hydrocarbon. Despite significant efforts by the State of Texas in improving BVOC estimates, the errors in emission inventories remain a concern. This is partly due to the diversity of the land use/land cover (LU/LC) over southeast Texas coupled with a complex weather pattern, and partly due to the fact that isoprene is highly reactive and relating atmospheric observations of isoprene to the emissions source (vegetation) relies on many meteorological factors that control the emissions, chemistry, and atmospheric transport.

BVOC emissions depend on Photosynthetically Active Radiation (PAR) reaching the canopy and temperature. However, the treatment of temperature and PAR is not uniform across emission models and still poses a problem when evaluating the emission inventories. Recent studies (e.g., Guenther et al., 2012) show that the largest source of uncertainty in BVOC estimates is the model solar radiation estimates and that using satellite-based PAR would be preferable. Emissions from soils also remain as one of the poorly quantified sources of nitrogen oxides (NOx) in most air quality models. Soils can be the largest source of NOx in rural regions where low-NOx conditions make ozone production efficiency especially high, contributing to background ozone levels.

Summary of the Project

This project specifically addressed two priority areas; namely improving biogenic emission estimates and improving the simulation of clouds in air quality models. In particular, a new satellite-based PAR estimate, retrieved from the Geostationary Operational Environmental Satellites (GOES) visible imager, for Texas was produced, evaluated, and used for BVOC estimates. The study episodes included selected periods of summer 2006 and September 2013. The 2013 period coincides with the Deriving Information on Surface Conditions from COlumn and VERtically Resolved Observations Relevant to Air Quality (Discover-AQ) Texas campaign. Also, a new soil NOx scheme, the Berkeley-Dalhousie Soil NOx Parameterization (BDSNP), which provides more mechanistic representation of how emissions respond to nitrogen deposition, fertilizer application, and changing meteorology, was incorporated into the Community

Multiscale Air Quality (CMAQ) model. BDSNP replaced the default Yienger and Levy 1995 (YL95) algorithm and was tested during the same periods. Furthermore, BDSNP was modified to be used as a stand-alone tool for estimating soil nitrogen monoxide (NO) emissions in any air quality modeling practice without conducting the atmospheric chemistry modeling. Stand-alone BDSNP along with a User's Manual will accompany this report.

The new satellite-based PAR product went through several iterations to fine tune the retrieval algorithm. The final product was evaluated against surface pyranometer observations from the Surface Radiation Budget Network (SURFRAD), the Soil Climate Analysis Network (SCAN), as well as Texas local broadband radiation monitoring stations for August 2006 and August-September 2013. The new PAR product was also compared against another satellite-based PAR product generated by the University of Maryland (UMD) (which is now discontinued) for August 2006. SURFRAD is operated by National Oceanic and Atmospheric Administration (NOAA) and is the only available direct continuous measurement of PAR at seven sites nationwide. SCAN is operated by the US Department of Agriculture and has continuous solar radiation measurements at more than 100 stations located in 40 states. In this project, 40 sites from the SCAN network, 7 sites from the SURFRAD network, and 47 sites from local Texas network were chosen to do performance evaluation of the satellite insolation/PAR retrieval products.

The new UAH PAR product was in good agreement with the UMD product. UAH product generally exhibited a small positive bias with respect to surface observations, while the UMD product showed a negative bias. However, both satellite retrieval products substantially outperformed Weather Research and Forecasting (WRF) model simulations. Compared to surface observations, correlation coefficients for satellite products were R=0.96~0.97 versus R=0.93 for the model. Satellite products also had smaller normalized mean error (NME) of 20.7%~20.1% compared to NME=35.5% for WRF. The UMD retrieval underestimated PAR with a normalized mean bias (NMB) of -12.4% while the University of Alabama in Huntsville (UAH) retrieval overestimated PAR with NMB of 10.2%.

Cloud assimilation in the Weather Research and Forecasting (WRF) model significantly reduced the normalized mean bias with respect to surface observations. NMB was reduced from 22.2% for control simulation to 8.9% for WRF with cloud assimilation. Additional evaluation of the results over 47 Texas Commission on Environmental Quality (TCEQ) sites (Broadband Radiation Monitoring networks) also indicated that cloud assimilation was able to significantly reduce the over-prediction by WRF. This result shows that WRF with cloud assimilation significantly improved the location and timing of clouds over Texas.

By using the new satellite-based PAR in the Model of Emissions of Gases and Aerosols from Nature (MEGAN), emission estimates indicated that the highest emission regions for isoprene in Texas are East Texas (2754 tons/day), North Central Texas (2036 tons/day), and Edwards Plateau (1199 tons/day). For terpenes, the highest emission regions are East Texas (1011 tons/day), Trans-Pecos (615 tons/day), and North Central Texas (562 tons/day). The results indicate that using GOES satellite retrievals on average reduced isoprene emission estimates by 20% and terpene emission estimates by 5% during August-September 2013 compared to the control case. In some regions these differences were as high as 29%. The emission algorithm for estimating terpenes in MEGAN is more impacted by the surface temperature than by PAR. The lowest emission estimates for terpenes over Texas were observed on August 15 and September 20 under overcast conditions.

Overall, the estimated isoprene emissions (for control case) by MEGAN resulted in simulated concentrations being 2-3 times higher than the observed values. Using satellite-based PAR reduced the emissions by about 30%. However, this reduction was not enough to correct the large model bias. The model was also unable to explain the observed diurnal variation of isoprene. The model results for isoprene in this project are consistent with findings from other AQRP investigations (e.g., AECOM project testing the sensitivity of different mechanisms to changes in BVOC emission estimates, or the University of Texas at Austin (UT Austin) project testing the impact of different land use/land cover on BVOC emission estimates). This suggests that the 2011 global BVOC emission factors in the current MEGAN release (v2.10), at least for isoprene, may have high uncertainty over Texas. Alex Guenther's group has been contacted with respect to this issue.

With respect to the other component of this project addressing soil NOx emission estimates, soil emission rates estimated by BDSNP module were consistently higher than the estimates by YL95 algorithm. The spatial patterns for the two algorithms were also quite different. YL95 estimated high NO emissions around Houston, while for BDSNP the highest emissions occurred near the state boundary between Texas, Louisiana and Arkansas. This contrast may be due to the combined contributions from different soil biome types, fertilizer implementations, and the different response curve for soil temperature and moisture in the two soil NO schemes. BDSNP estimated 674 moles/s over the East Texas region. This estimate is about 2.3 times higher than the corresponding YL95. But for South Texas, YL95 estimates were about 3 times higher than BDSNP (34.8 moles/s for YL95 versus 12.9 moles/s for BDSNP). Overall, the estimates by BDSNP were about 21% higher than YL95 over Texas. The stand-alone BDSNP module along with the user's manual accompanies this final report.

A series of CMAQ simulations was also performed to evaluate the impact of emission and meteorological changes on air quality predictions. The base case used the MEGAN outputs derived by default WRF simulation, the case marked "analytical" in this report used the MEGAN outputs derived by WRF simulation with cloud assimilations, and the case named “UAHPAR” used the MEGAN outputs derived by satellite PAR retrievals and the soil NO emission from BDSNP scheme. The preliminary results from these simulations do not show a significant difference in ozone predictions. Compared to observations from 38 evaluation sites over Texas the correlation coefficients were around 0.75-0.76. The base case overestimated ozone concentration by 2-3%, which is consistent with previous modeling studies (Song et al., 2008; Kota et al., 2015). By using the cloud assimilation in WRF, the ozone performance was marginally better, decreasing the mean bias from 2.8% to 2.4%, the root mean square error (RMSE) from 14.5 ppbV to 14.2 ppbV, and the NMB from 18.2% to 17.0%. Model performed better over the Dallas-Fort Worth metroplex (DFW) region with correlation coefficients of 0.75-0.77 and NME of 28.9%-30.6%. On average, the model underestimated mean ozone over Austin, DFW, East Texas and El Paso regions while overestimating mean ozone over Corpus Christi, HGB and San Antonio regions. The ozone predictions over Corpus Christi exhibited the highest NMB in all three simulations (105-111%).

Due to the large bias in biogenic VOC emission estimates by MEGAN, even after a 30% reduction in BVOC emissions (resulted from using satellite data) most of the modeling domain over east Texas was saturated with VOC and remained sensitive to NOx. Therefore, the CMAQ simulations used in this study did not show a substantial improvement in ozone prediction over east Texas. These simulations should be repeated using a biogenic emissions model that better represent clear sky emission estimates.