AQRP Monthly Technical Report

PROJECT TITLE	Improving Modeled Biogenic Isoprene Emissions under Drought Conditions and Evaluating Their Impact on Ozone Formation	**PROJECT #**	14-030
PROJECT PARTICIPANTS	Qi Ying, Gunnar W. Schade, John Nielsen-Gammon, Huilin Gao	**DATE SUBMITTED**	2/9/2015
REPORTING PERIOD	**From:** January 1, 2015 **To:** January 31, 2015	**REPORT #**	7

A Financial Status Report (FSR) and Invoice will be submitted separately from each of the Project Participants reflecting charges for this Reporting Period. I understand that the FSR and Invoice are due to the AQRP by the 15th of the month following the reporting period shown above.

Detailed Accomplishments by Task
Task 1: Meteorology simulation with WRF. Completed.

Task 2: Perform field and laboratory measurements on common Texas tree species
Note: Due to an additional project start delay from June to July and the unanticipated need to move all our seedlings to a different greenhouse in July, all monthly milestones described in the QAPP had to be moved by one month ahead

The January milestones were addressed as follows:

a. compare baseline to treatment measurements: Greenhouse measurements were conducted mid-January, but the plants were found to remain seasonally dormant, meaning they show negligible photosynthesis and isoprene emissions. Greenhouse seedlings were monitored for pests and watered when necessary.
b. analyze observed drought responses of seedlings and field-grown mature trees: No additional analyses on greenhouse seedling data have been carried out. However, we have (i) begun to assemble the 2001 field data in a way conducive to analyzing the effects of the 2011 Texas drought on observed leaf-level isoprene emissions, and (ii) carried out another required cartridge test for the activated carbon adsorbent cartridges. Retesting was performed to determine the change of (isoprene) sample when cartridges are stored in the laboratory. The length of this test was 4 days, while typical storage time in any of our experiments did not exceed 48 hours. Test conditions were similar to the test described in our last monthly reported, but sample size was larger (500 mL) for these cartridges than for the Tenax ones (200 mL). In addition, we tested "non-cleaned" cartridges. i.e. cartridges that had not been run through the pre-measurement day cleaning cycle. The test showed that (i) cartridge cleaning is important to lower a cartridge's background, since diffusion over time can lead to significant accumulation of VOCs on a cartridge; and (ii) the change of concentration of isoprene over time is significantly less than 5%, and thus does not represent a significant error in need of correction in our sampling and analysis work-flow.

The results are summarized in Figure 1.

Further, shown in Figure 2 is the progression of standard ("basal") isoprene emission (1000 PAR units illumination, 30 °C leaf-T) from our 2011 field experiments in the Houston metro area. It is showing isoprene emissions and variability (1 SD error bars) throughout the season with clear responses to the regional drought as it progresses throughout the summer. However, low topsoil moistures in the spring did not affect isoprene emissions, probably due to available deep soil moisture in the spring, while higher topsoil moistures late in the season did not lead to a recovery of isoprene emissions, possibly due to a lack of deep soil moisture at that time. This obviously requires further analysis.

c. submit data files to UT: we attached a new data format for approval (TCEQdata_new_format.xlsx)

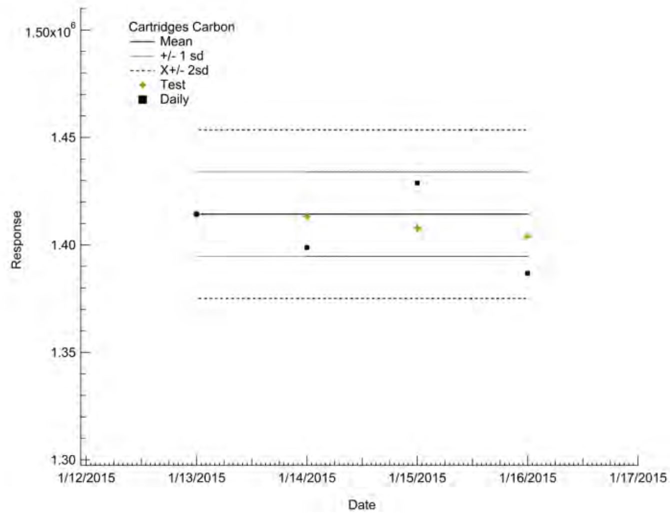

Figure 1: FID area response development for the isoprene peak from stored vs. freshly loaded carbon adsorbent cartridges using an isoprene mixing ratio of approximately 25 ppb (500 mL sample size), similar to what is typically found in cartridges taken from seedling leaves in the greenhouse.

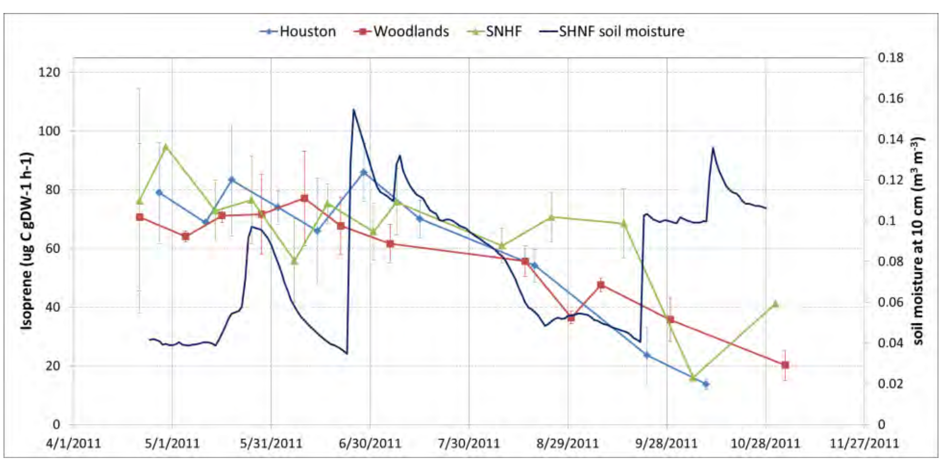

Figure 2: Basal isoprene emissions from post oaks in the field during 2011 (field days showing averages ±1 sd, connected by lines) alongside measured (average daily) topsoil moisture (continuous measurement at nearby weather station)

Task 3: Evaluate drought parameterization for isoprene emissions – Not started yet.

Task 4: Perform regional BVOC modeling using MEGAN – Completed. Both base case and the drought parametrization case have been completed for all three domains.

Figure 2 shows that emissions of isoprene are predicted to reduce significantly with the current drought parameterization in July and August. Changes in September emission rates are small. In contrast, based case isoprene emission rates in 2007 are significantly lower and soil moisture does not significantly influence isoprene emissions, indicating a relatively wet year.

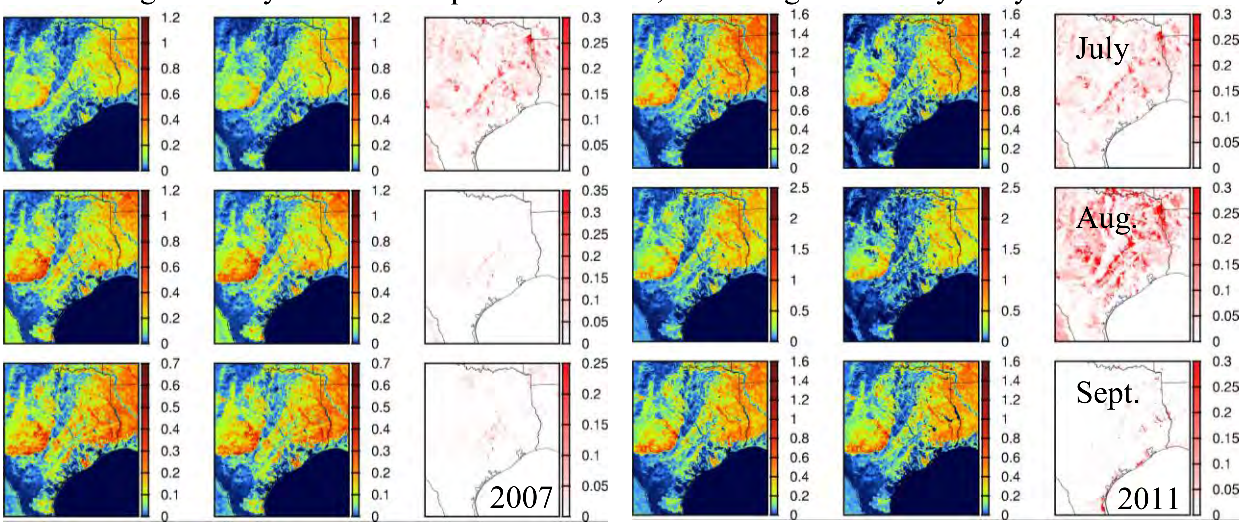

Figure 3: Monthly average isoprene emissions for July (first row), August (second row) and September 2007 and 2011 for the 4-km Texas domain. First column shows base case emissions rates, second column shows emission rates with drought parameterization and last column shows the different in isoprene emission rates. Units are mol/s.

Task 5: Perform regional air quality simulations

CMAQ simulations were conducted for 2011 for both emission scenarios. The 36-km and 12-km runs have been completed and 4-km simulations are on-going. Reduced isoprene emission greatly affected regional ozone concentrations. Figure 4 shows an example of predicted regional ozone concentrations with and without drought parameterization. In some areas, especially in downwind areas of major urban areas, differences in peak hour ozone concentrations can be as high as 30-40%. Model performance analysis will be presented in the Preliminary Analysis section.

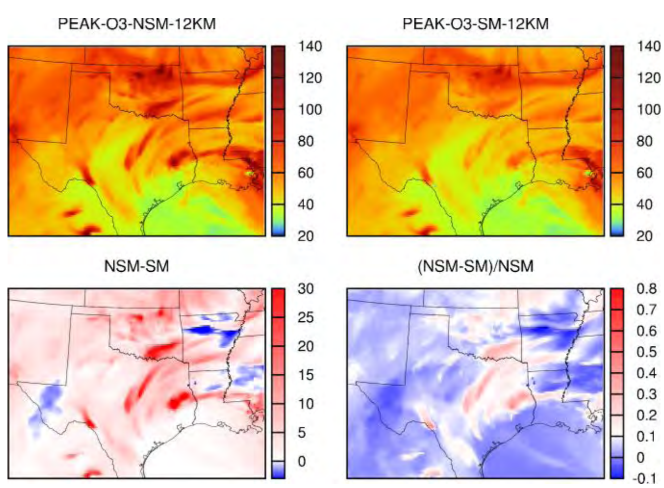

Figure 4: Peak hour (1400 CST) ozone concentrations on August 12, 2011. NSM: Base case simulation without soil moisture correction. SM: simulation with drought parameterization. Units are ppb, except for the relative difference.

Preliminary Analysis

Task 2: Figure 1 shows that no significant losses of isoprene are observed from the cartridges. Laboratory air testing is ongoing to evaluate if diffusion into the cartridges from there is the possible culprit of seemingly increasing isoprene levels during the first test, and increasing background contamination observed on non-cleaned cartridges. Results will be reported next month.

Task 5:
We looked at ozone model performance in Texas based on the 12-km simulations. For May 2011, CMAQ simulated ozone concentrations generally agree with observations at all auto-GC sites, and most other TCEQ operated monitors throughout Texas, as shown in Figures S1-S4. However, model performance decreases significantly as emissions of isoprene start to increase in later months. Figure S5-S8 shows time series of ozone for August 2011, and predicted concentrations are much higher than observations, even with reductions due to drought parameterization.

This poor ozone performance appears to be associated with large over predictions of isoprene emissions by the MEGAN model in the region, as it has been reported previously. Table 1 shows the observed and predicted August monthly average isoprene concentrations at all Auto-GC sites with available data. At all stations except one, the base case simulation over predicted isoprene concentrations by 3.55-38.3 times, with a mean over-prediction of 9.6 times. The drought parameterization greatly reduced the isoprene concentrations but still shows an average over prediction by a factor of 2.8. Additional comparison of daily average isoprene with PAMS data should be carried out to check the spatial extent of the over-prediction problem.

Table 1: Observed and predicted isoprene concentrations at the Auto-GC sites for August 2011. SM and NSM are for simulations with and without drought parameterizations. Units are ppb.

Station	Obs.	Pred. (SM)	Pred. (NSM)
481350003	0.02	0.06	0.25
482010026	0.49	0.57	1.74
482010069	0.26	0.41	1.14
482010617	0.19	0.62	1.35
482011015	0.12	0.89	1.44
482011035	0.41	0.40	1.73
482011039	0.27	0.65	1.65
482450009	0.36	0.71	1.24
482451035	0.33	0.82	1.16
481410044	0.03	0.12	1.15
481130069	0.03	0.18	0.19
481211007	0.58	0.19	0.49
484390075	0.07	0.21	2.45
484391002	0.09	0.28	0.74
484970088	0.25	0.30	1.02
483550083	0.13	0.46	0.52

Data Collected

1. 3rd set of cartridge tests: Cartridge isoprene contents as a function of time for fixed isoprene mixing ratio collected, and for blanks

Identify Problems or Issues Encountered and Proposed Solutions or Adjustments

Based on our preliminary analysis, MEGAN appears to over-predict isoprene concentrations during summer months of 2011. Ozone over-predications are likely associated with isoprene emissions. We plan to 1) apply BEIS 3.14 for 2011 using default input data and see if it can reasonably predict isoprene concentrations. Our previous study using BEIS shows more reasonable isoprene predictions on August 2006 at a number of Auto-GC sites in Texas, as shown in Figure 5. We will also examine our MEGAN input files and make sure no mistakes were made during emission processing. We would also like to compare MEGAN predictions made independently by other research groups as an additional cross check.

If it is confirm that MEGAN indeed over-predicts isoprene emission based on the current input data, we plan to apply a general scaling factor to bring the predicted isoprene in agreement with observations for the current project. Additional analysis of MEGAN input data should be carried out to isolate the problem(s).

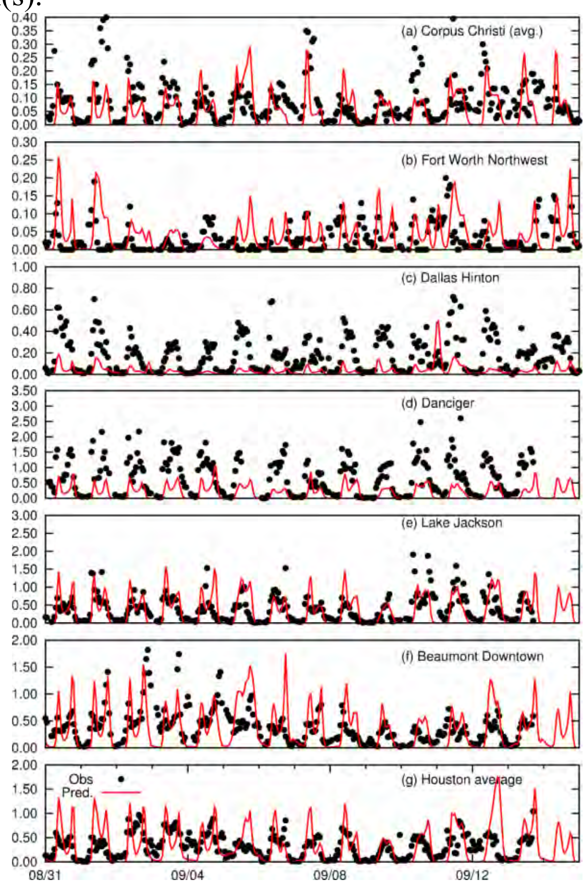

Figure 5: Predicted and observed isoprene at some Auto-GC sites for September 2006, based on BEIS 3.14 emissions. (Ying et al. 2015, Significant Contributions of Isoprene to Summertime Secondary Organic Aerosol in Eastern United States, Submitted for review)

Goals and Anticipated Issues for the Succeeding Reporting Period

Goals

Task 2: 1) derive a better estimate of total, or a depth profile of soil moisture data during the 2011 field season in order to better relate isoprene emissions to soil moisture; 2) continue caretaking of the greenhouse-based seedlings, monitoring potential new growth as ambient insolation increases; monitor newly acquired post oak and other seedling for growth: we have obtained a new set of seedlings from a different provider, who uses a different growth technique to assure higher vitality; seedlings were planted into the same soil mix, fertilized and watered, and are stored alongside the "old" seedlings in the greenhouse, awaiting leaf-out.

Task 5: 1) perform additional isoprene observation vs. prediction analyses for daily isoprene at PAMS sites to check the extent of the isoprene over-prediction problem; 2) generate biogenic emissions using BEIS 3.14 in SMOKE (BEIS does not currently employ a drought parameterization scheme), and compare predicted isoprene emission rates with MEGAN predictions; and compare ozone and isoprene predictions with observations; 3) perform additional sensitivity runs to see if other biogenic emissions, especially monoterpene needs to be scaled due to drought with the same scaling factor applied for isoprene, and see if it affect ozone performance.

Detailed Analysis of the Progress of the Task Order to Date

Task 1: Completed.

Task 2: Due to the delayed start of the project and ongoing issues, we are one to two months behind schedule (see proposed solution above and in last two reports).

Task 3: Waiting for a new drought parameterization but this would not slow down the progress of the project.

Task 4: Completed.

Task 5: Isoprene over-predictions and ozone model performance problems need to be resolved. We still have plenty of time complete the CMAQ runs if the problem can be isolated and fixed next one or two months.

Submitted to AQRP by: Qi Ying

Principal Investigator: Qi Ying

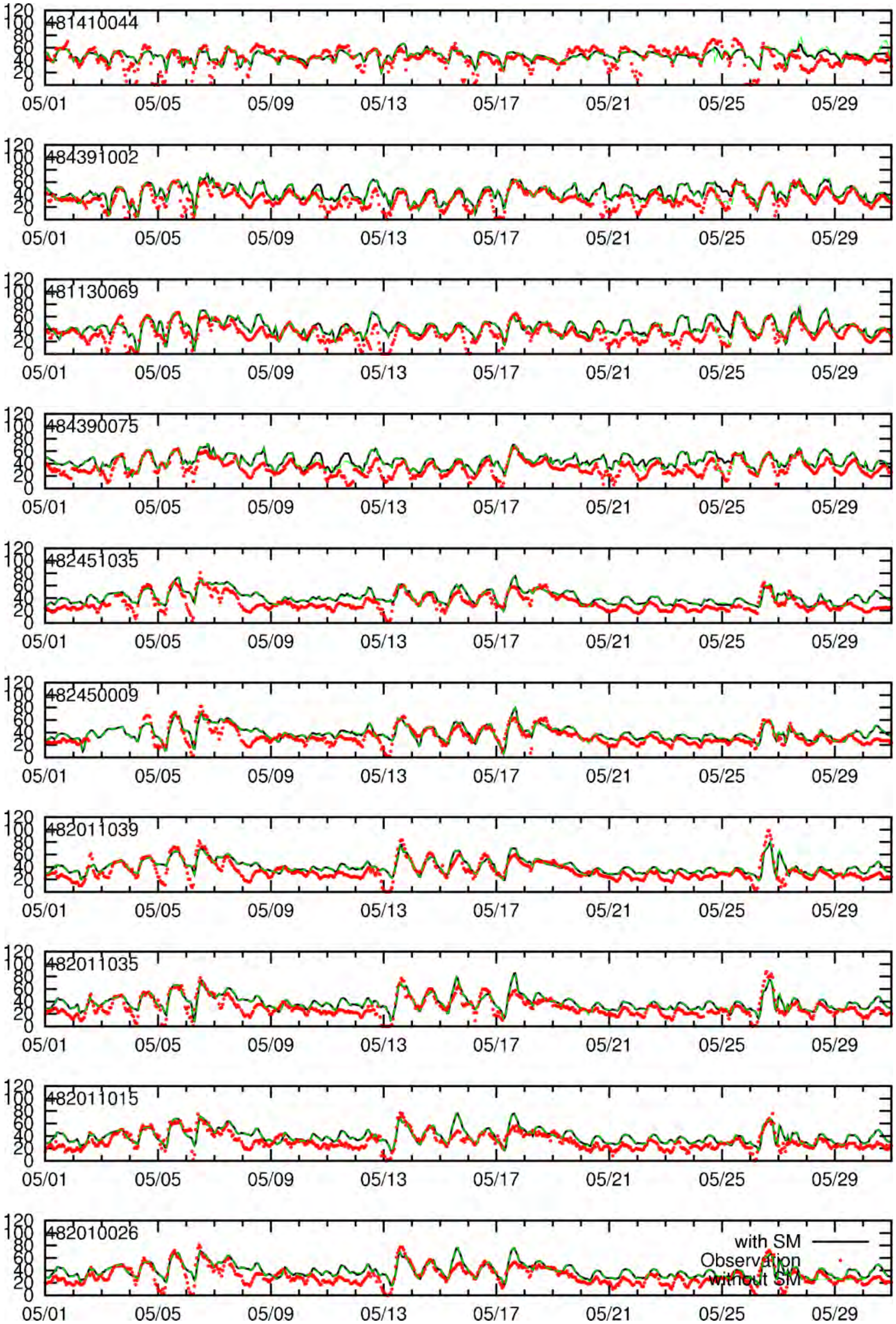

Figure S1: Predicted (based on 12-km resolution results) and observed ozone concentrations at Auto-GC sites in May 2011. Red dots are observations; green lines are base case predictions and black lines are predictions with drought parameterization applied for isoprene emissions. Units are ppb.

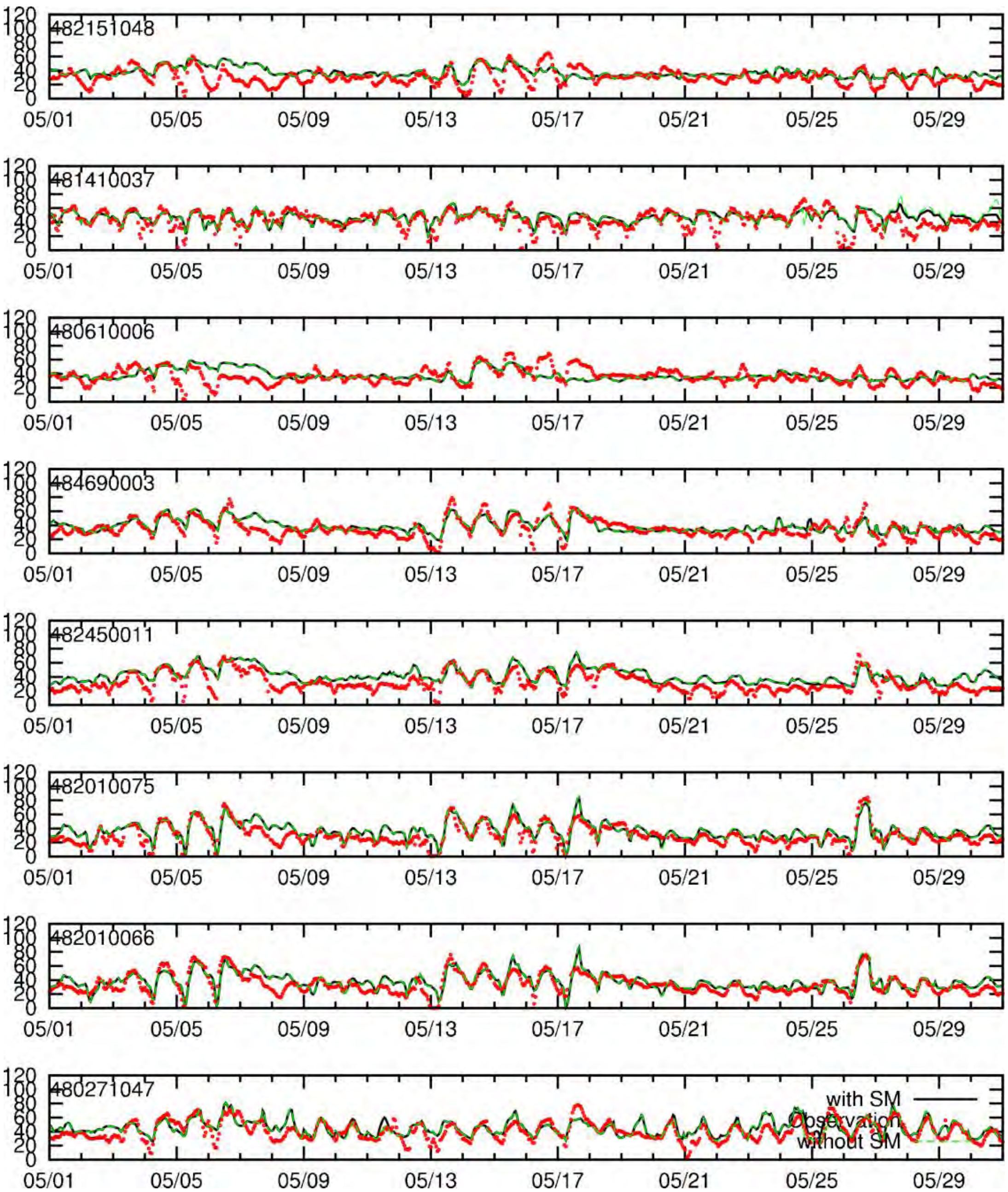

Figure S2: Same as Figure S1, for other TCEQ sites at urban locations. Units are ppb.

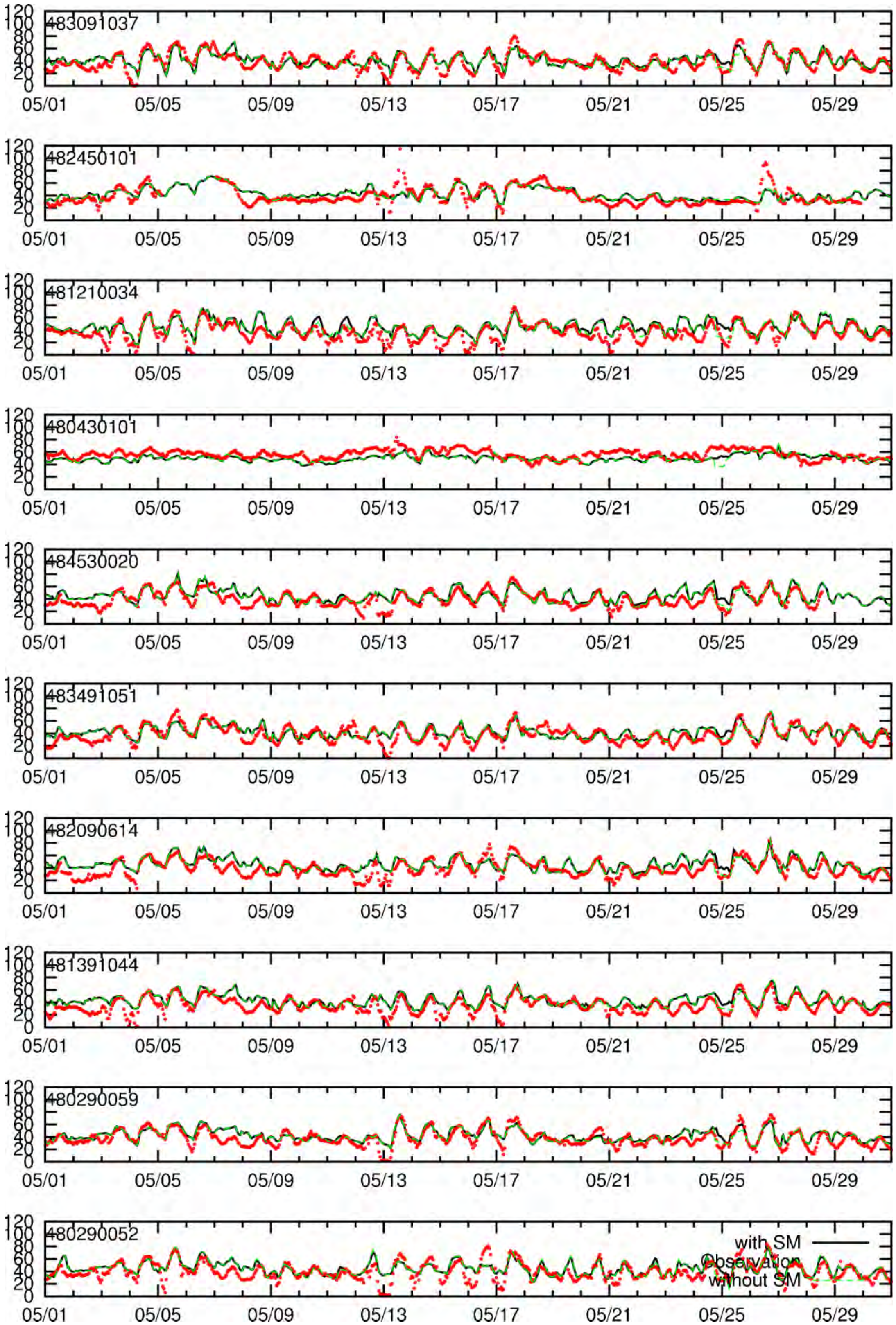

Figure S3: Same as Figure S1, for other TCEQ sites at rural locations. Units are ppb.

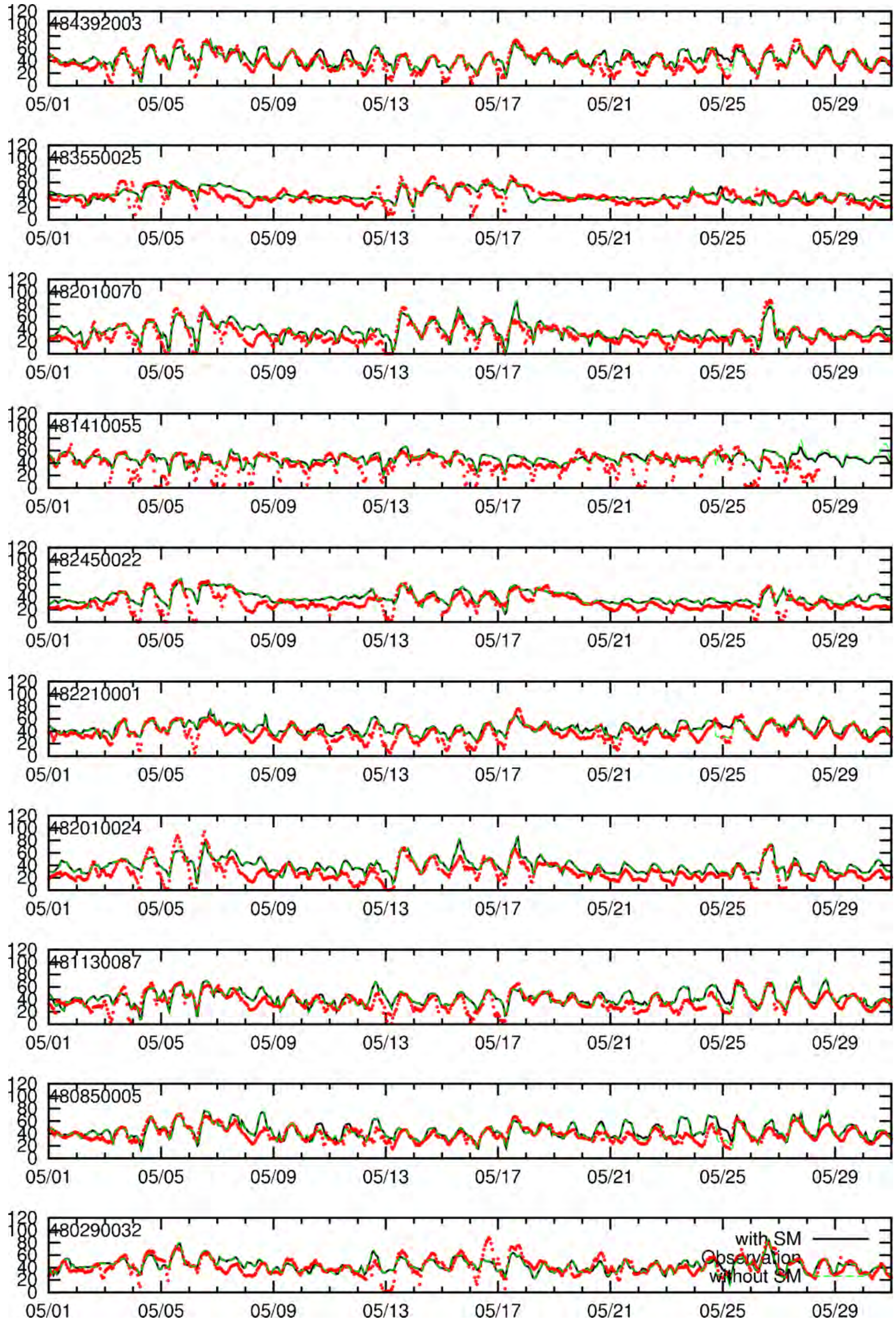

Figure S4: Same as Figure S1, for other TCEQ sites at suburban locations. Units are ppb.

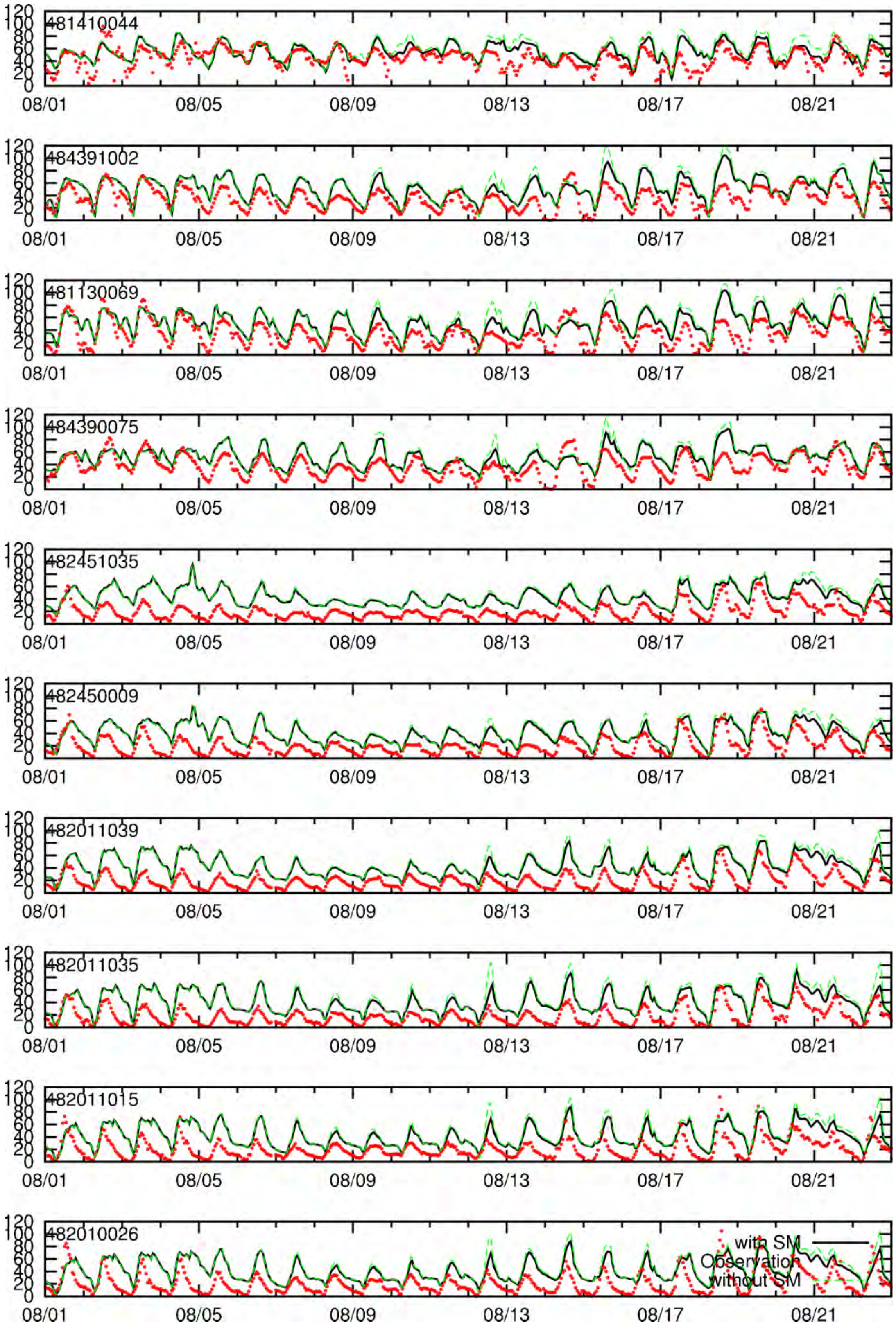

Figure S5: Predicted (based on 12-km resolution results) and observed ozone concentrations at Auto-GC sites in August 2011. Red dots are observations; green lines are base case predictions and black lines are predictions with drought parameterization applied for isoprene emissions. Units are ppb.

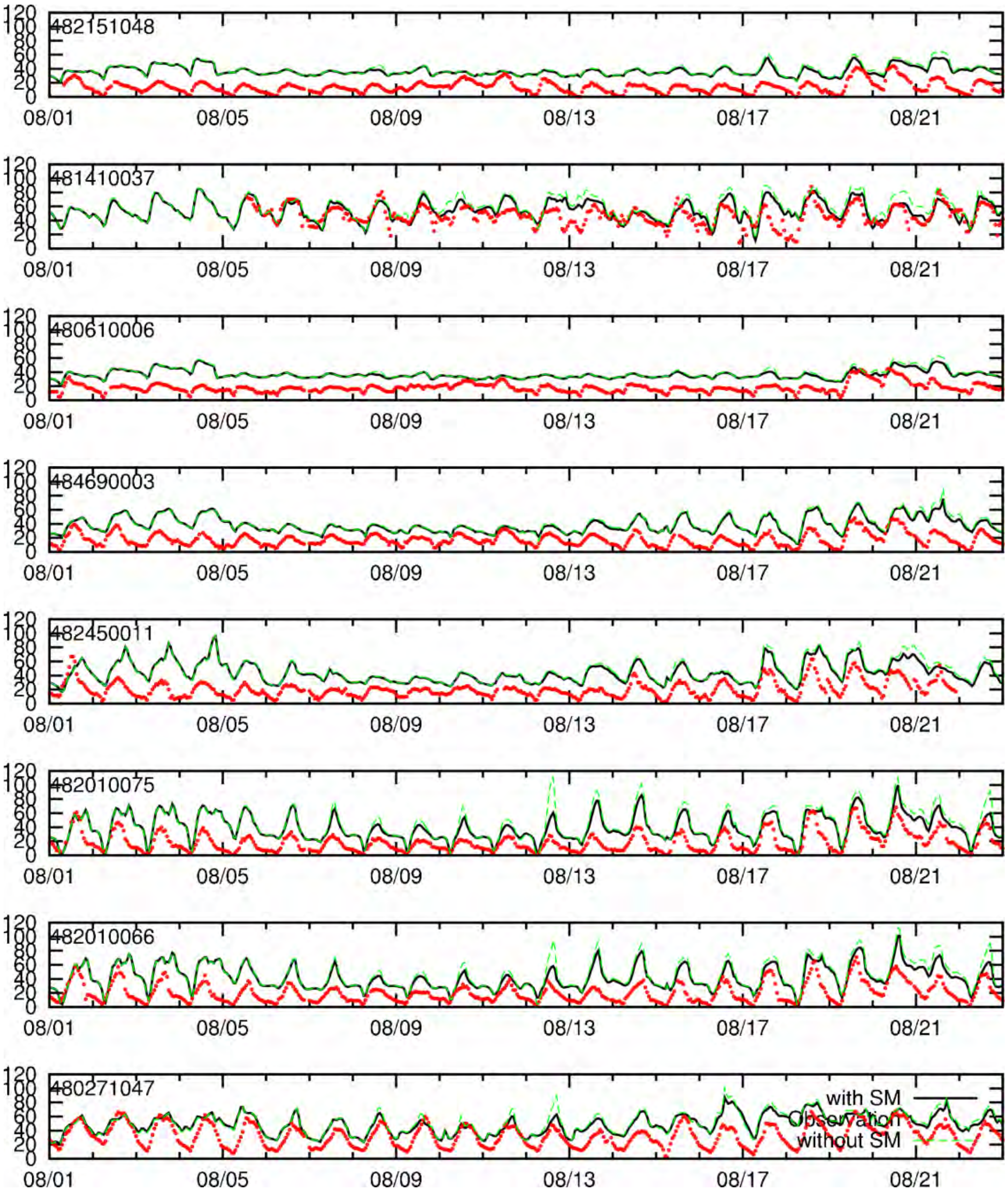

Figure S6: Same as Figure S5, for other TCEQ sites at urban locations. Units are ppb.

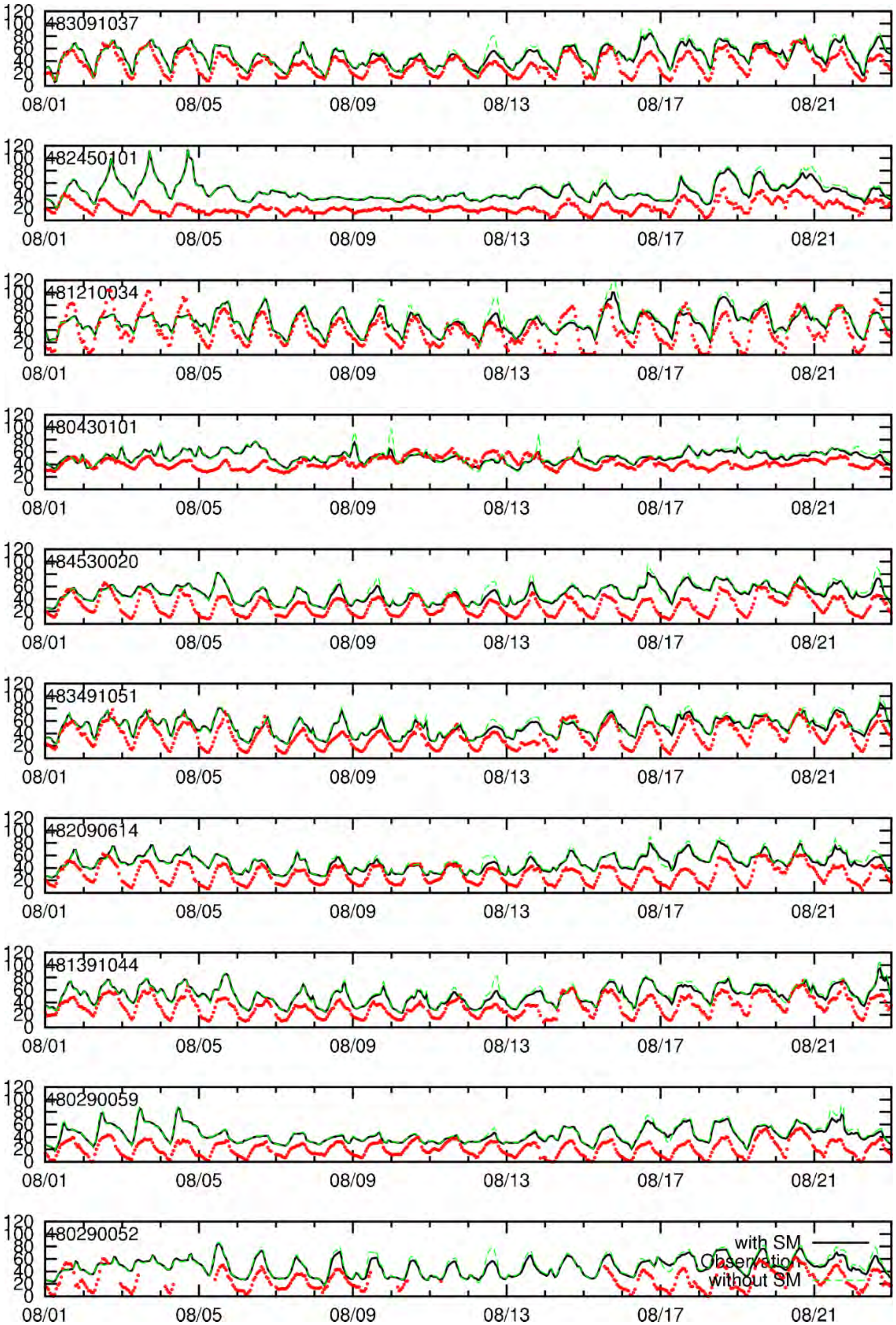

Figure S7: Same as Figure S5, for other TCEQ sites at rural locations. Units are ppb.

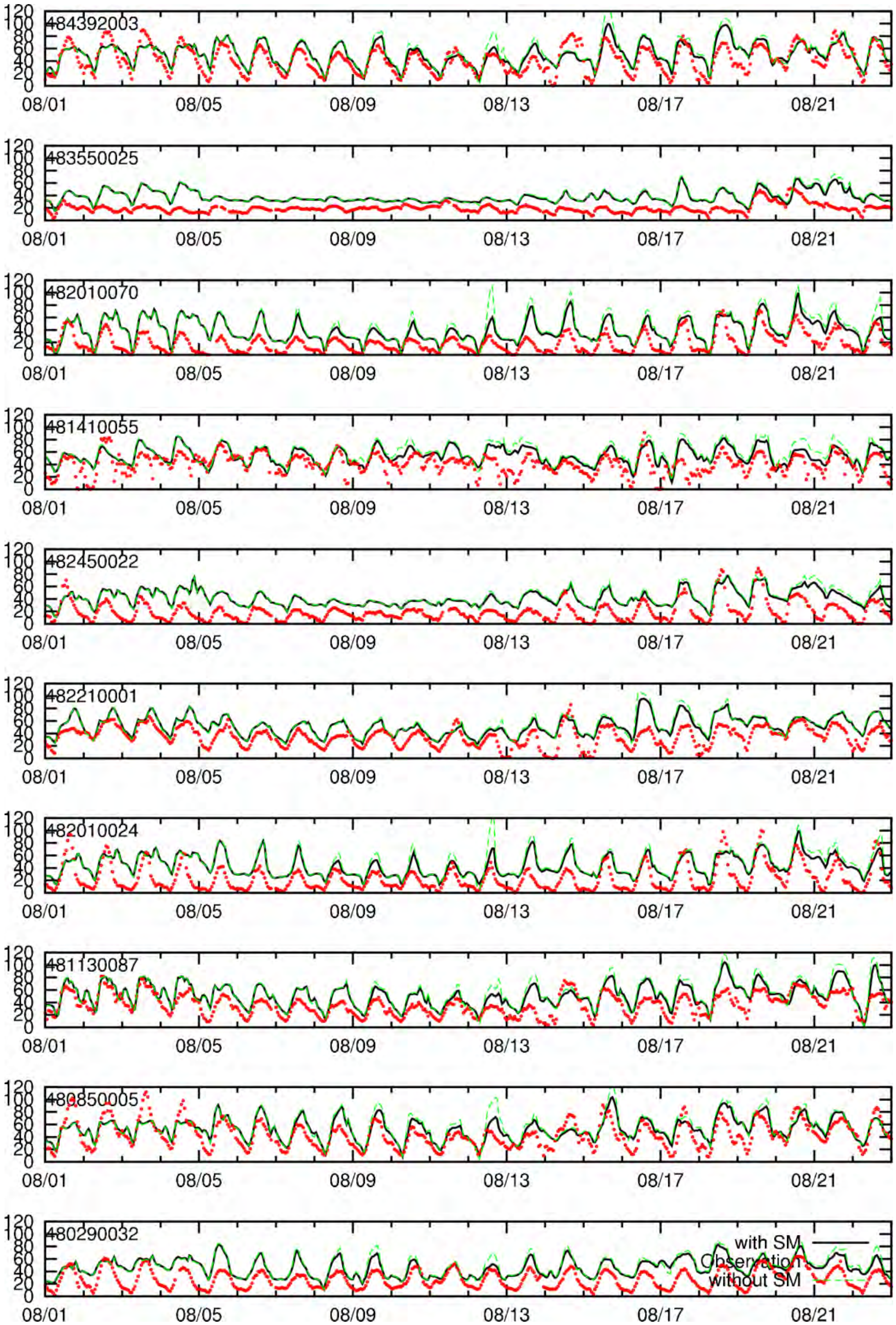

Figure S8: Same as Figure S5, for other TCEQ sites at suburban locations. Units are ppb.