AQRP Monthly Technical Report

PROJECT TITLE	A synthesis study of the role of mesoscale and synoptic-scale wind on the concentrations of ozone and its precursors in Houston	PROJECT #	10-010
PROJECT PARTICIPANTS	Qi Ying, John Nielsen-Gammon	DATE SUBMITTED	12/10/2018
REPORTING PERIOD	**From:** 11/1/2018 **To:** 11/31/2018	REPORT #	2

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: Synthesis of mesoscale wind structures in the synoptic-scale context

Work on Task 1 has focused on identifying synergies and opportunities for leveraging personnel and computer resources. We are collaborating with Prof. Yangyang Xu of Texas A&M and his graduate student, who are engaged in a research project with the National Center for Atmospheric Research (NCAR) to track transport of Central American biomass burning aerosols across the Gulf of Mexico using WRF-CHEM. For the AQRP project, they are planning to extend the domain northward from their original plan and to run the meteorological model (WRF) an extra few months, to provide meteorological simulations for most if not all of the 2017 warm season. We will use this simulation to obtain a WRF climatology of wind rotation and recirculation, to determine whether the model properly reproduces the patterns of wind change in time and space, and to identify candidate good-performing episodes for WRF-driven CMAQ simulations.

Task 2: Development of source and age-resolved CMAQ

We incorporated the source-resolved SAPRC-99 mechanism developed in the previous month into a condensed version of the SAPRC-07 mechanism (CS07A, https://www.cert.ucr.edu/~carter/SAPRC/files.htm). CS07A uses the SAPRC-99 peroxy radical representation. This is the most condensed version considered appropriate for airshed model calculations. It reduces gas phase computation time by approximately 20% when 10 sources of primary VOCs, HCHO, NOx, and O_3 are tracked in the simulation. The source-oriented CS07A mechanism implemented in CMAQ and the CMAQ model is further modified to track the atmospheric age of the primary VOCs, NOx, and O_3.

Task 3: Analysis of the interaction of mesoscale winds and ozone formation during key episodes
None to report.

Preliminary Analysis

The source/age resolved CS07A mechanism for 10 sources has 299 species and 1223 reactions. In comparison, the SAPRC99 mechanism with 10 sources has 399 species and 1372 reactions. The computation efficiency of the CS07A is again tested using the two-day episode from TexAQS2006 on a 10-core/20-thread E5-2670 v2. Only 8 cores were requested for these simulations. The gas phase computation time for the CS07A is approximately 82% of the SAPRC-99 mechanism (see Figure 1).
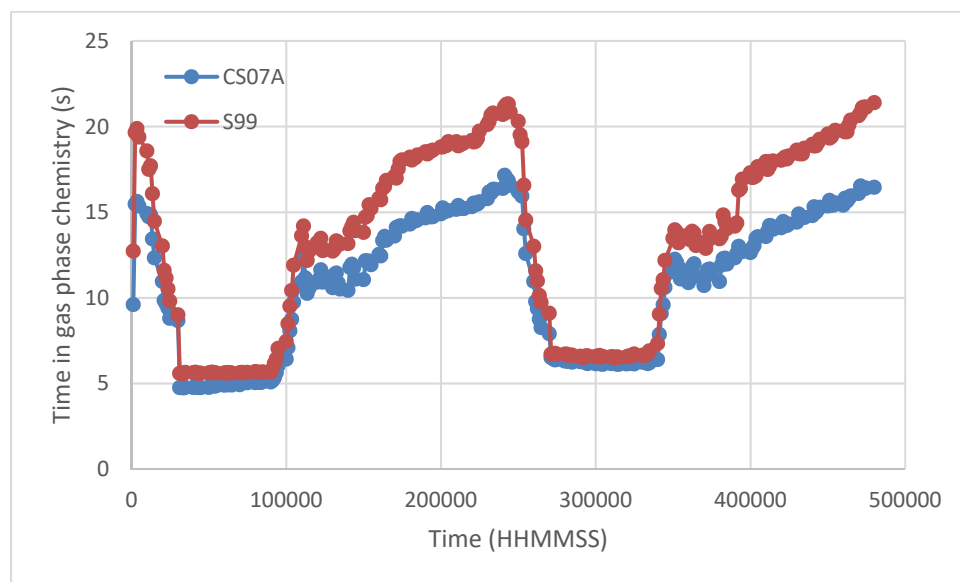
Figure 1 Wall-clock time for gas phase chemistry at each time step during the two-day simulation (August 28-29, 2006) using the condensed SAPRC-07 (CS07A) and the SAPRC-99 for 10-sources. All simulations were performed on a 10-core/20-thread E5-2670 v2. Only 8 cores were requested for these simulations.

Data Collected
None to report.

Identify Problems or Issues Encountered and Proposed Solutions or Adjustments
None to report.

Goals and Anticipated Issues for the Succeeding Reporting Period
We plan to use the age-resolved for CS07A to study atmospheric age of ozone and its precursors during TexAQS2000 and TexAQS2006 as a preliminary application of the age-resolved mechanism. Regarding Task 1, we plan to obtain, process, and begin analysis of the wind profiler observations.

Detailed Analysis of the Progress of the Task Order to Date
While the project has a late official start, we have made sufficient progress that in time completion is expected.

Do you have any publications related to this project currently under development? If so, please provide a working title, and the journals you plan to submit to.

_X__Yes   ___No

We are working on a manuscript with a preliminary title "Improve the computation efficiency of source-oriented chemical mechanisms for the source apportionment of secondary gaseous and particulate pollutants", which we plan to submit to Atmospheric Environment.

Do you have any publications related to this project currently under review by a journal? If so, what is the working title and the journal name? Have you sent a copy of the article to your AQRP Project Manager and your TCEQ Liaison?

___Yes   __X_No

Do you have any bibliographic publications related to this project that have been published? If so, please list the reference information. List all items for the lifetime of the project.

___Yes   _X__No

Do you have any presentations related to this project currently under development? If so, please provide working title, and the conference you plan to present it (this does not include presentations for the AQRP Workshop).
___Yes   _X__No

Do you have any presentations related to this project that have been published? If so, please list reference information. List all items for the lifetime of the project.

___Yes   _X__No

Submitted to AQRP by Qi Ying, on December 10, 2018.

Principal Investigator