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	11/09/2018
REPORTING PERIOD	From: 10/26/2018 To: 10/31/2018	REPORT #	1

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
None to report so far.

Task 2: Development of source and age-resolved CMAQ

We improved the computation efficiency of the source-oriented approach for the source apportionment of ozone. In previous source-oriented models, the chemical reactions and number of model species increase quadratically with the number of sources or source sectors. In the improved method, the number of reactions and number of model species increase linearly with the number of sources/sectors, thus greatly improved the computation efficiency. In addition, a new ozone source apportionment scheme is included so that the model is capable of simultaneously track ozone from a large number of sources or source sectors simultaneously. The ozone source apportionment scheme is a three-regime scheme that correctly considers in-situ ozone formation in the transition regime. A manuscript is being prepared to document this. This work is done based on SAPRC-99 and currently, we are also trying to incorporate these changes into SAPRC-07.

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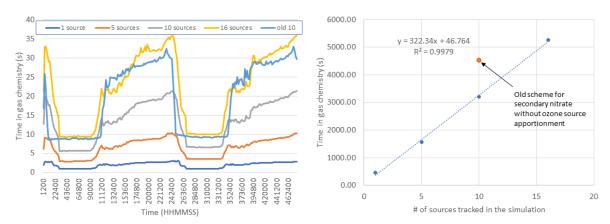
Preliminary Analysis

The improved ozone source apportionment scheme was tested using a two-day episode from TexAQS2006 to evaluate its computation efficiency and scalability. The following table shows the number of model species, reactions, and time spent in gas-phase chemistry for the two-day simulation using a 10-core/20-thread E5-2670 v2. Only 8 cores were requested for these simulations. The number of species, reactions and computation time all scales almost linearly with the number of sources.

Table 1 Number of model species, reactions and gas-phase chemistry time for source-oriented mechanisms with increasing number of simultaneous sources

# of sources	Species	Ratio	Reactions	Ratio	Time (s)	Ratio
1	90	1.000	226	1.000	466.12	1.000
5	229	2.544	752	3.327	1560.43	3.348
10	399	4.433	1372	6.071	3207.34	6.881
16	603	6.700	2116	9.363	5268.02	11.302
Old 10*	331	3.678	1772	7.841	4644.00	9.963

* An old source apportionment scheme that tracks 10 sources of NOx and their products for secondary nitrate source apportionment. Primary VOCs, HCHO and ozone were not tracked in that mechanism.

Figure 1 shows more details of the computation time for the gas-phase chemistry. Figure 1(a) shows the time spent in gas-phase chemistry at each time step for four sets of simulations with 1, 5, 10 and 16 sources, respectively, and Figure 1(b) shows the total amount of time in the gas-phase chemistry for these simulations. The computation time records for an old source apportionment scheme that tracks 10 sources of NOx and their products for secondary nitrate source apportionment are also included for comparison. The new scheme that includes source apportionment of NOx, SO2, NH3, primary VOCs, HCHO, and ozone for 10 sources needs only 70% of the time of the old scheme yet generates much more information.

Figure 1(a) Wall-clock time for gas phase chemistry at each time step during the two-day simulation (August 28-29, 2006) for simulations with a different number of sources (including the vanilla type) and (b) total wall-clock time for the gas phase chemistry part of the two-day simulation. Units are seconds. 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 develop a source- and age-resolved for SAPRC-07 based on this work for SAPRC-99. We will also further improve the mechanism so that it can track the age distribution of ozone from multiple sources/source regions simultaneously.

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 November 9, 2018.

Principal Investigator