AQRP Monthly Technical Report

PROJECT TITLE	The Influence of Alkyl Nitrates from Anthropogenic and Biogenic Precursors on Regional Air Quality in Eastern Texas	**PROJECT #**	16-019
PROJECT PARTICIPANTS	University of Texas at Austin (Drs. McDonald-Buller and Hildebrandt Ruiz) Ramboll Environ (Dr. Yarwood)	**DATE SUBMITTED**	6/8//2017
REPORTING PERIOD	**From:** 5/1/2017 **To:** 5/31/2017	**REPORT #**	8

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: Refinements to the CB6r4 Mechanism in CAMx

CAMx v6.40 with the SOAP2r3 scheme is serving as the base case for simulations that evaluate updates to the CB6r4 mechanism. The team completed documentation of the results of the CAMx performance evaluation with SOAP2r3 and comparisons with the SOAP2 and the 1.5-D VBS schemes as part of final project report.

Updates have been made to the CB6r4 mechanism resulting in new versions for sensitivity studies. A summary of new CB6 versions is provided below:

- **CB6r4 with τ = 3 h or τ = 1 h pseudohydrolysis of NTR2.** As described in the previous monthly technical report, the CB species NTR2 represents organic nitrates that can partition significantly to organic aerosol. The gas-particle partitioning of NTR2 and subsequent hydrolysis of NTR2 in the particle phase are implemented as a pseudo gas-phase reaction in CAMx v.6.40. In the base case, the particle-phase NTR2 hydrolysis lifetime is set to 6-hours according to Liu et al. (2012). Sensitivity studies were conducted that reduced the particle-phase NTR2 hydrolysis lifetime in the CB6 mechanism to 1-hour or 3-hours with no other changes relative to the base case.
- **CB6r6d1.** Terpenes were differentiated into two classes, α-pinene represented by the new model species APIN and other terpenes represented by the existing model species TERP. This version of the mechanism also assumed rapid pseudohydrolysis of NTR2 with τ = 1 h.
- **CB6r6d4.** This version includes all updates that were part of CB6r6d1. In addition, the alkane chemistry (i.e., the CB6 model species PAR) was revised to differentiate lighter from heavier alkanes.

Application of the CB6r6d1 or CB6r6d4 mechanisms required modifications to the base case emissions inventory. For CAMx simulations with CB6r6d1 or CB6r6d4, α-pinene was split

from other terpenes, such that the TERP species in the CB mechanism was split into APIN and TERP. For the CAMx simulation with CB6r6d4, PAR emissions were split into PAR and PARH using the split factors shown in Table 1.

Table 1. Split factors applied to the base case PAR inventory to obtain PAR/PARH inventory.

PAR:PARH	Source Category
0.8:0.2	On-road/Non-road/Off-road
0.85:0.15	Area/Mexico_Canada/Low Point/Elevated_Point_Anthro
0.9:0.1	Oil_Gas
1.0:0.0	MEGAN/FINN_fires (i.e., no change for these categories)

Task 2. Evaluating CB6r4 Updates in CAMx Modeling for DISCOVER-AQ
CAMx simulations are being performed with the mechanism updates. Two simulations have been completed that consider only changes to the pseudohydrolysis lifetime for NTR2 (τ = 3 h or τ = 1 h) in CB6r4. A CAMx simulation has also been completed with the CB6r6d1 mechanism. These three CAMx simulations are identical to the base case except for the changes to the gas-phase chemical mechanism. Analyses of the results are ongoing.

CAMx simulations that investigate the effects of the CB6r6d4 mechanism are ongoing. Our initial focus has been primarily on the impacts to predicted ozone concentrations and consequently we have not included the aerosol chemistry in these simulations. We have invoked the Decoupled Direct Method (DDM) tool in these simulations, as well as for the base case, to examine ozone sensitivity to emissions from different source sectors that have different PAR/PAH splits, e.g. urban, oil and gas, natural (biogenic and fires).

Task 3. Project Reporting and Presentation
On-going per requirements.

Preliminary Analysis
As above.

Data Collected
None.

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

Goals and Anticipated Issues for the Succeeding Reporting Period
The objective by the next reporting period is to complete all of the CAMx simulations described above. Output from the simulations with varying pseudohydrolysis lifetimes for NTR2 and the simulation with the CB6r6d1 mechanism will be evaluated relative to the base case. We will analyze the results of the base case and CAMx simulation with the CB6r6d4 mechanism with the DDM tool invoked when they are complete. We will continue to work on drafting the final project report.

Detailed Analysis of the Progress of the Task Order to Date
The project is proceeding as planned.

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.

___Yes __X_No

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

Elena McDonald-Buller