AQRP Monthly Technical Report

PROJECT TITLE	Quantifying the Emissions and Spatial/Temporal Distributions of Consumer Volatile Chemical Products (VCPs) in the Greater Houston Area	**PROJECT #**	22-020
PROJECT PARTICIPANTS	Dr. Yue Zhang, Alana Dedero, Sahir Gagan, Sining Niu, Dr. Ying Qi, Hee Won Yim	**DATE SUBMITTED**	07/10/2023
REPORTING PERIOD	**From:** 6/1/2023 **To:** 6/30/2023	**REPORT #**	10

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 for reporting period

1. Completed the data analysis for the trace gases (Vocus) and the particle phase chemical composition (AMS) for both the fall and winter campaigns.
2. Completed instrument calibration analysis of trace gases (Vocus)
3. Generating 6 major VCP concentrations as a function of their GPS coordinates
4. Started to compare seasonal difference of the VCPs
5. Setup CAMQ model to simulate the fall campaign.

Data Collected

1. We have collected a full suite of data of the trace gases (Vocus), particle phase chemical composition (AMS), CO, NO_2, O_3, aerosol size distribution, GPS location through our deployment around Houston, Rockport, Corpus Christi, San Antonio, and Austin.
2. We have collected the above gas and particle information both during the day and at night, during weekends and weekdays, and on sunny, cloudy, rainy days, and during the fall and winter.
3. We also have collected Vocus data both in ammonia (NH_4^+) mode and water cluster (H_3O^+) mode.
4. We have obtained the organic concentration of particle phase compounds and have identified concentrations for VCPs for both the fall and winter campaigns.
5. We have identified concentrations for 61 different VCP compounds for the fall and winter campaigns.

Identify Any Problems or Issues Encountered and Proposed Solutions or Adjustments

N/A

Goals and Anticipated Issues for the Succeeding Reporting Period

1. Dr. Zhang's lab finished the initial data analysis for all data collected from both the Fall and Winter field campaigns for all 6 VCP tracers, and performed quality assured (QA) and quality checked (QC) on all data.
2. Currently Dr. Zhang's lab is pairing data with GPS locations and send such data for Dr. Ying Qi's CAMQ model.
3. In addition, Dr. Zhang's lab starts to compare seasonal differences of the fall and winter campaign.
4. Dr. Qi Ying's lab finishes setting up the CMAQ model simulation for the fall campaign, and now integrating data into the CAMQ model to refine the VCP concentrations.

Based on the current progress, both goals are on track.

Detailed Analysis of the Progress of the Task Order to Date

We completed the initial data analysis to determine spatial trends of VCPs in the Houston area for the six major VCP tracers. Now we are comparing the fall and winter deployments to understand the seasonal variation of VCP and the impact vegetation has on VCP concentrations. We will identify the factors impacting days of high concentrations and areas with high concentrations. We will additionally compare the field measurements with CMAQ model simulations. The Table below lists the data we have quality assured (QA) and quality checked (QC) for uploading to the data archive that was described in the QAPP.

Table 1: Data that passed QA/QC for analysis and data archive.

Fall			**Winter**		
Date	*Route*	*Ionization Mode*	*Date*	*Route*	*Ionization Mode*
10/30	Round	NH_4^+	1/12	North-South	NH_4^+
11/02	East-West	NH_4^+	1/13	Round	NH_4^+
11/04	Round	NH_4^+	1/14	Round	NH_4^+
11/05	North-South	H^+	1/15	East-West	NH_4^+
11/06	Round	H^+	1/17	Round	H^+
11/07	Round	H^+	1/18	Round	H^+
11/09	East-West	H^+	1/19	North-South	H^+
			1/21	East-West	H^+
			1/22	North-South	H^+
			1/23	Round	H^+
			1/24	North-South	H^+

Dr. Qi Ying's lab has crossed referenced with Dr. Zhang's lab and added all available VCP compounds to their simulations, as shown in Table 2. The read

Table 2 Model and Measurement Data Comparison

Model Nnme	Analytical standards used	Example uses/sources of all listed isomers
	D5-siloxane	Cosmetic products, antiperspirants
	Triethylene glycol	Automobile fluids, lubricants, solvents
	Ethyl acetoacetate	
	Furfural	Feedstock chemical, specialty solvent, wood off- gassing, biomass burning
ETGLYCL	**Ethylene glycol hexyl ether; 1,2 Octanediol**	
CC6KET	**Cyclohexanone**	Solvent for paints, degreasers, polymers, etc.
	Hydroxycitronellal	Fragrances, solvents, insect repellants
TEXANOL	**Texanol**	Paint solvent, other solvents
	Acetophenone	Automobile exhaust, fragrances
	Benzyl acetone	Perfumery, cosmetic products
	Pentadioic acid, dimethyl ester	Fragrances
PGMEACT, CSVACET	**PGMEA; 2-Ethoxyethyl acetate**	Coatings, printing inks, deicing formulations
DPGOME2,ETOETOH	**1-Methoxy-2-propanol**	Industrial solvent
IBUACET,BUACET, DIACTALC	**Butyl acetate**	Fragrances, paints, solvents
BUOETOH, M24C5OH2	**2-Butoxyethanol**	Solvents, cosmetic products, coatings, surfactant stabilizer
PRGLYCL	2-Methoxy ethanol; **Propylene glycol**	Solvent for varnishes, dyes, wood stains
DGBE	2-(2-Butoxyethoxy)ethanol; **DGBE**	Paints, inks, surface cleaners, varnishes
	6-Methyl 5-hepten-2-one	Skin oil oxidation product, fragrances
	Propyl paraben	Cosmetics
	Maltol	Dyes, other industrial processing, food additive
	Dimethyl pthalate	Insect repellents, lacquer coatings, plastics
	Cyclopentanone	Precursor to fragrances, flavoring agent
MEK, THF	**Methyl ethyl ketone**	Paints, dyes, adhesive remover, degreasers, solvent
MNBK	**2-Hexanone; 4-Methyl-2-pentanone**	Solvent
	Phenoxy ethanol	Fragrances, soaps
NMP	**Methyl pyrrolidone**	Industrial solvent
BZCH2OH	**Benzyl alcohol**	General solvent
	Ethyl paraben	Cosmetics
DPRGLCL (isomer), DGEE	**Dipropylene glycol**	Industrial solvent, paints, wood stains, textile inks, brake fluids
MEMACRT	**Methyl methacrylate**	Solvents for paints, inks and lacquers, coffee aroma
ACET, RCHO	**Acetone**	Wide-use solvent, disinfectant
MVK, MACR, CROTALD	**Methyl vinyl ketone**	Chemical precursor
	Butyl paraben	Antioxidant, cosmetic preservatives

IPRACET, PRACET	**Isopropyl acetate; n-Propyl acetate**	Fragrances, industrial solvent
BALD	**Benzaldehyde**	Soaps, dyes, fragrances
	Methyl paraben	Cosmetics, personal care products
	Menthol	Fragrances, insect repellants, food flavoring
DETGLDL	**Diethylene glycol**	Solvent for resins, dyes, oils
	Eugenol	Fragrances, cosmetic preservatives, food flavoring, consumer products
	Diethyl phthalate	Plasticizer in consumer products
	TXIB	Inks, coatings, lacquers
	Dipropylene glycol propyl ether	Industrial solvent, inks, coatings
	Acetonitrile	Industrial solvent, chemical precursor, combustion by-product
MEACET, RCOOH	**Methyl acetate; Propionic acid**	Industrial solvent, naturally occurring
	Cyclohexyl acetate	Flavoring agent, fragrances
	Benzyl acetate	Fragrances, food flavoring
	2-Phenoxyethyl isobutyrate	
ETACET	Butyric acid; **Ethyl acetate**	Industrial solvent, coatings, fragrances, food flavoring
	Methyl benzoate	Fragrances
CARENE3, APINENE, BPINENE, DLIMONE, SABINENE	**Monoterpenes**	Widely-used fragrances, Food flavoring, biogenic sources
	Benzoic acid	Fragrances, dyes, insect repellents
	Octanoic acid	Disinfectants, skin products, industrial solvent
SIOME4	**D4 siloxane**	Adhesives, silicone rubbers, gels
	Methyl octanoate	Fragrances, cigarette additive
SESQ	**Sesquiterpenes**	Fragrances, biogenic sources
ETGLYCL	**Ethylene glycol**	Antifreeze, coolant, de-icing agent, paints, printing inks
VINACET	**Vinyl acetate**; Methyl acrylate	Monomer, precursor/feedstock, nail primers, fragrances
GLYCERL	**Glycerol**	Personal care products, foods

Dr. Qi Ying's lab also has finished setting up the CMAQ model for the fall campaign period. They used all TCEQ sites for model validation. Results have shown that CO, O_3, and VOC gas concentrations agree well between the model and the measurement. Currently, Dr. Qi Ying's lab is working on assimilating the data from the field data to the model. Figure 1-6 below show the modeling results. Dr. Ying's lab performed data validation for more than 20 different species. Due to limit of pages, we only listed 6 species.

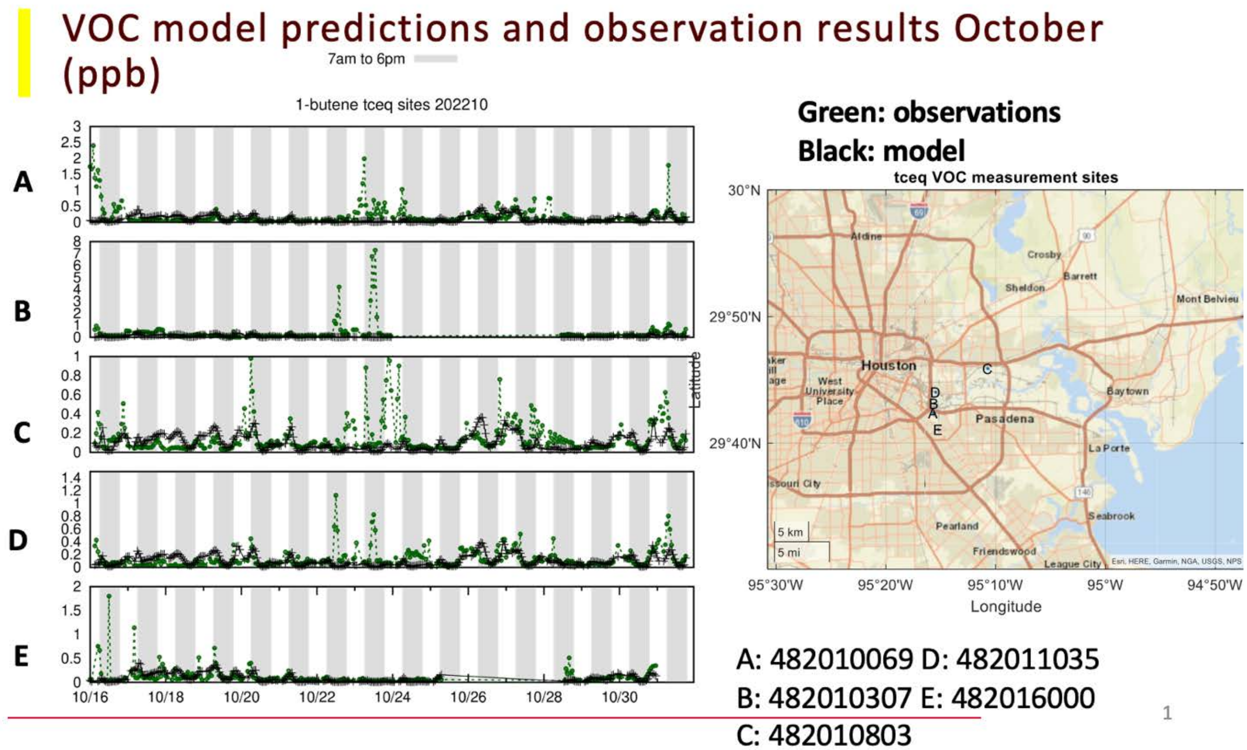

Figure 1. Validation of 1-butene between CMAQ Modeling Results and Measurement data from TCEQ sites A-D.

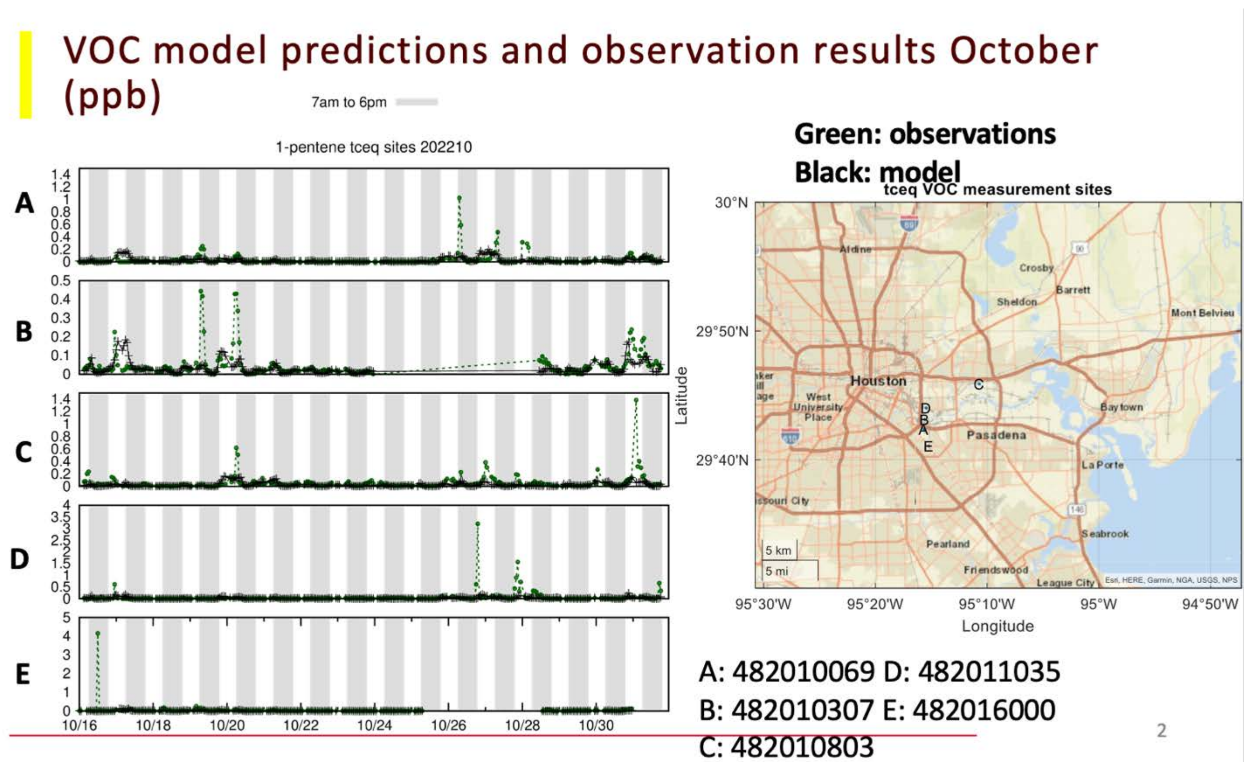

Figure 2. Validation of 1-pentene between CMAQ Modeling Results and Measurement data from TCEQ sites A-D.

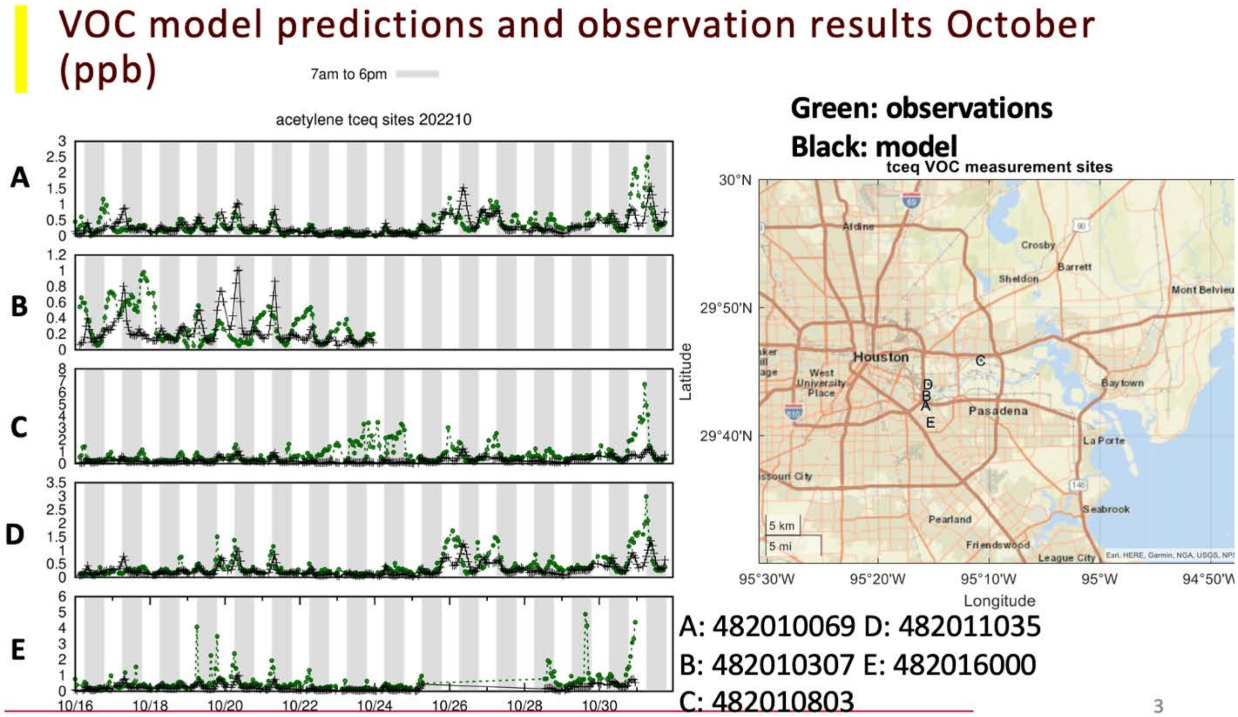

Figure 3. Validation of 1-acetylene between CMAQ Modeling Results and Measurement data from TCEQ sites A-D.

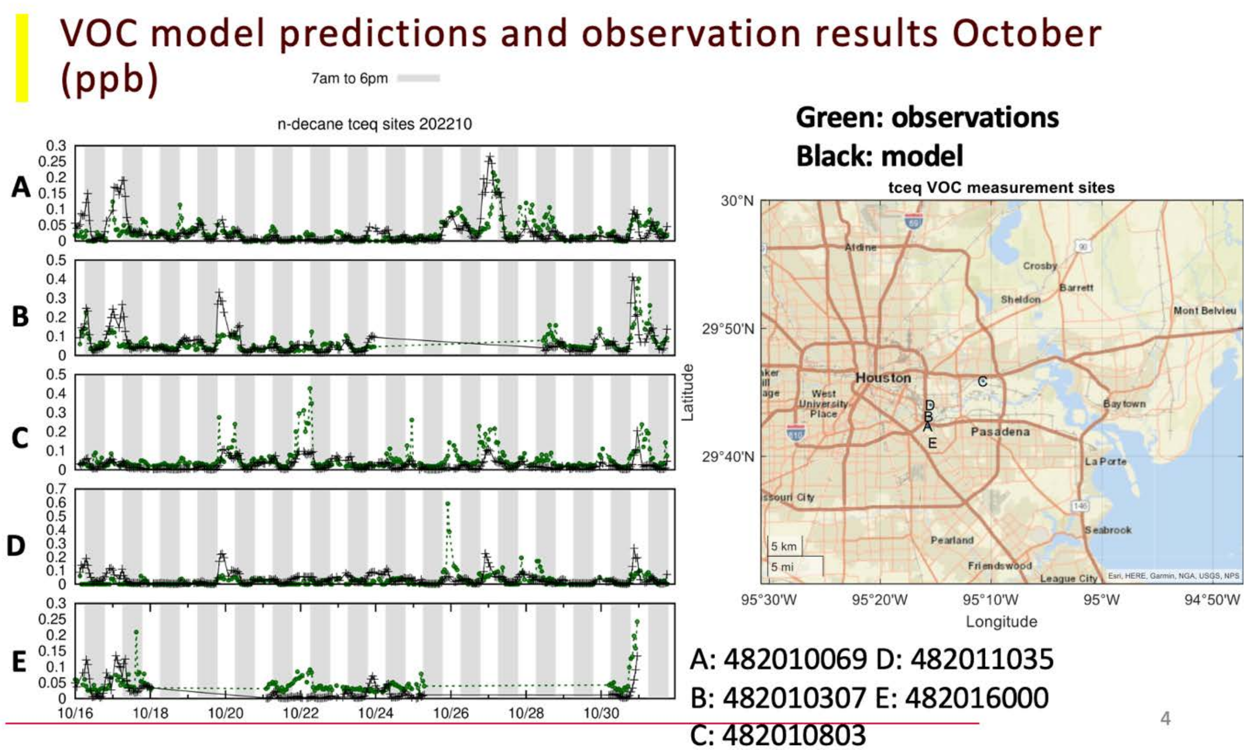

Figure 4. Validation of 1-decane between CMAQ Modeling Results and Measurement data from TCEQ sites A-D.

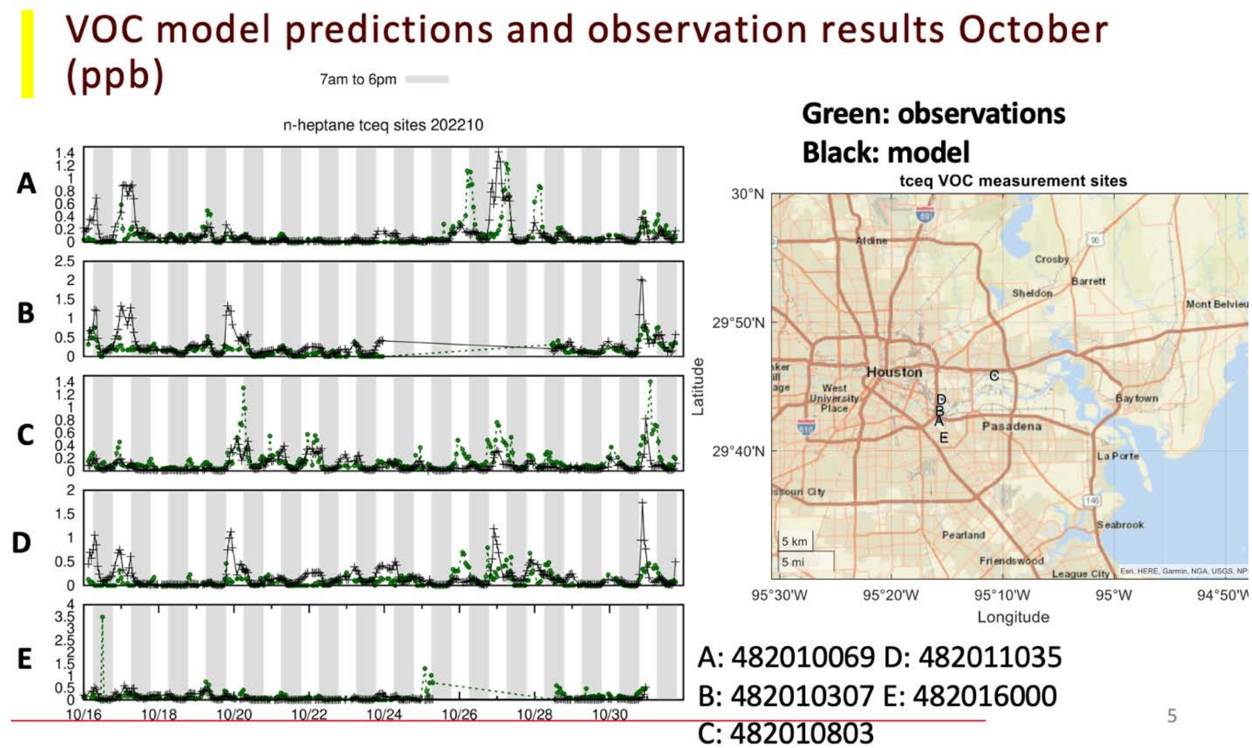

Figure 5. Validation of 1-heptane between CMAQ Modeling Results and Measurement data from TCEQ sites A-D.

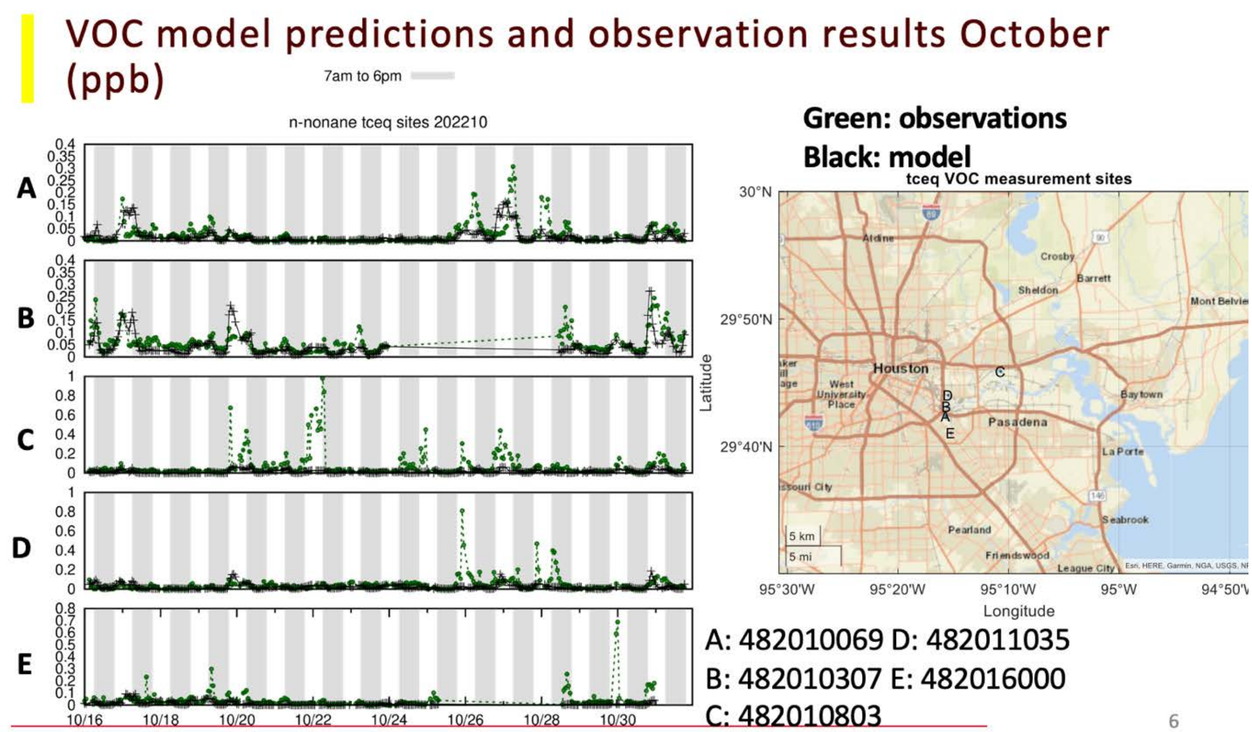

Figure 6. Validation of 1-nonane between CMAQ Modeling Results and Measurement data from TCEQ sites A-D.

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** ☒ **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** ☒ **No**

Do you have any bibliographic publications (ie: publications that cite the project) 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** ☒ **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** ☒ **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** ☒ **No**

Have any personnel changes occurred that were not listed in the original proposal? If so, please include a detailed description of the personnel change(s) below.

☐ **Yes** ☒ **No**

Are any delays expected in the progress of the research? If so, please include a detailed description of the potential delay below.

☐ **Yes** ☒ **No**

Describe any possible concerns/issues (technical or non-technical) that AQRP should be made aware of.

Are you anticipating using all the available funds allocated to this project by the end date? If not, why and approximately what is the amount to be returned?

☒ **Yes** ☐ **No**

The whole funding is expected to be used by the end of the project date.

Submitted to AQRP by Dr. Yue Zhang