

Prepared for:

Texas Commission on Environmental Quality  
12100 Park 35 Circle MC 164  
Austin, TX 78753

Prepared by:

Ramboll  
7250 Redwood Blvd., Suite 105  
Novato, California 94945

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# VOC Speciation Update for Point Sources Modeling

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**VOC Speciation Update for Point Sources Modeling  
Final Report**

Ramboll  
7250 Redwood Boulevard  
Suite 105  
Novato, CA 94945  
USA

T +1 415 899 0700  
<https://ramboll.com>

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## Executive Summary

Volatile Organic Compounds (VOC) are precursors to ozone and fine particulate matter which causes regional haze. Thousands of individual compounds make up the VOC emissions reported by regulated entities and tracked within the State of Texas Air Reporting System (STARS). When the Texas Commission on Environmental Quality (TCEQ) conducts photochemical modeling for the Texas State Implementation Plan (SIP), it is important to properly characterize the air quality impacts of VOC emissions. This requires an accurate mapping of the VOC compounds present in the inventory to the model species used by air quality models.

This project aimed to improve how VOCs emitted by Texas point sources are represented in the TCEQ's SIP modeling by updating compound mappings and incorporating new nationally recognized standard speciation profiles from the EPA. Key updates included enhancing two critical components: (1) speciation profiles that specify the weight fraction of individual VOCs emitted by each source, and (2) the compound database mapping individual VOCs to model species of the CB7 chemical mechanism used by photochemical models like CAMx.

We updated the compound mappings to include intermediate-volatility organic compounds (IVOC) model species and explicitly map alpha-pinene to the APIN model species, thereby transitioning the STARS mapping from CB6 to CB7. Additionally, we added many new EPA standard VOC speciation profiles from the latest version of the SPECIATE (v5.3) database to TCEQ's standard VOC speciation library. These updates are pivotal steps toward more precise air quality modeling and improving secondary organic aerosol (SOA) predictions.

# 1 Introduction

## 1.1 Background

Accurate speciation of Volatile Organic Compound (VOC) emissions is crucial for understanding air quality impacts of emission sources in photochemical modeling. When the TCEQ conducts air quality modeling for the Texas State Implementation Plan (SIP), it is important to properly characterize VOC emissions using appropriate chemical speciation profiles. This conversion process transforms total VOC emissions from the inventory into model species required by regional air quality models through a step known as 'speciation' in the emissions processing. As new speciation information becomes available, the TCEQ's emissions processing procedures must be updated accordingly.

Facility-specific speciated VOC emission data is available in the State of Texas Air Reporting System (STARS) and can be utilized for air quality modeling by mapping STARS VOC compounds to chemical mechanism model species (e.g., Carbon Bond) used by the Comprehensive Air quality Model with extensions (CAMx). However, the current mechanism mappings used by the TCEQ do not take into account intermediate-volatility organic compounds (IVOCs) which are significant contributors to secondary organic aerosol (SOA) formation.

## 1.2 Project Objectives

This project aims to achieve the following objectives:

1. Update Mechanism Mapping: Incorporate IVOC model species into the mechanism mapping for the STARS and explicitly map alpha-pinene to the APIN model species. These updates will transition the STARS mapping from CB6 to CB7.
2. Upgrade EPA Standard VOC Speciation Profiles: Update the EPA standard VOC speciation profiles used in point source processing. This upgrade is important for improving VOC emissions characterization in air quality modeling.
3. Assist TCEQ in Impact Assessment: Support the TCEQ in evaluating the impacts of the updated mechanism mappings and speciation profiles on emissions input for air quality modeling. This assessment will help ensure that the updated VOC speciation files are functioning as intended.

## 2 Development of Point-Specific Speciation Profiles

The STARS database contains total and speciated VOC emissions for each point source in Texas. Companies that operate major point sources in Texas must submit total VOC emissions and are encouraged to also report speciated VOC emissions to STARS every year. STARS is a valuable source of VOC speciation data for use in TCEQ's SIP modeling but there are data processing challenges to integrate partially reported VOC speciation data with the remaining portion of total VOC emissions.

The TCEQ has developed a unique processing methodology that considers each point source individually and retains all reported speciated VOC data and, if the speciated data sum to less than total reported VOC, characterizes any remaining unspeciated VOC by using EPA speciation profiles (Cantu, 2003; PES, 2001). The processing approach is implemented in a SAS script along with QA/QC activities such as removing any non-VOC species before processing and splitting generic chemical mixtures reported by industry (such as "crude oil" or "gasoline") into component hydrocarbons using existing chemical profiles. The resulting point-specific VOC speciation profiles are used for emissions processing with EPS3 to prepare emission inputs for SIP modeling. EPS3 uses the point-specific profiles and cross-reference information to convert inventory VOC into model species of the photochemical mechanism.

As new information becomes available for VOC speciation, the TCEQ's emissions processing procedures need to be updated. Two types of information are required to conduct VOC speciation: (1) profiles that specify the weight fraction of individual VOCs emitted by each source type, and (2) the mechanism mapping that defines how individual VOCs are assigned to the model species of chemical mechanism (e.g., Carbon Bond version 7, CB7) used in the photochemical model (e.g., CAMx).

In this project, we updated the compound mappings, reviewed the EPA speciation profiles used by the SAS script to characterize unspeciated VOC emissions, and updated these profiles where newer information was available. Ramboll and the TCEQ worked collaboratively to complete the project with Ramboll updating data files and the TCEQ running the SAS script that uses the updated data files. The next section describes how these updates were carried out.

### 3 Methodology

The TCEQ provided current versions of data files that are used by the SAS script to create point-specific VOC speciation profiles. This includes the current EPA VOC weight fraction profiles (emscvt.std\_profiles.tog.24Apr2019) and the existing mechanism mappings for the CB6 chemical mechanism (compound\_database.cb6\_final.23Apr2019.txt). Each of these data inputs and updates are described in detail below.

#### 3.1 Updating EPA VOC Speciation Profiles

The unspiciated portion of the VOC emissions for each point source is speciated using EPA standard VOC speciation profiles. Each emission point is assigned a standard speciation profile from EPA based on its reported Source Classification Code (SCC) according to an EPA SCC-Speciation Profile cross-reference.

EPA curates a comprehensive database of speciation profiles in the SPECIATE database which is updated periodically as new profiles become available from measurement studies. Upon reviewing TCEQ’s current standard VOC speciation data, we determined that many profiles needed updating to newer profiles available from the most recent version of the SPECIATE database (v5.3; EPA 2024).

We identified 129 new profiles for point sources that can be added based on EPA’s 2016v3 platform (2016gf) speciation cross-reference file (Eyth, 2022). These profiles were integrated into the existing file “emscvt.std\_profiles.tog.24Apr2019” using the method outlined in the previous Ramboll report titled “VOC Speciation Update for Texas Point Sources” (Ramboll, 2019). Each Species ID was padded with leading zeros to create a 5-character long SAROAD code in the compound database.

Table 1 shows the distribution of updated standard VOC profiles by source category. While every source category listed in Table 1 has at least one representative profile, certain categories feature multiple profiles to capture subcategory nuances. Furthermore, we updated the cross-reference file for standard profiles used by the SAS script, incorporating EPA’s 2016v3 cross-reference files for point sources. This update included existing entries as well as hundreds of new SCCs identified in EPA’s files but were previously absent from the TCEQ cross-reference file.

We provided the updated files “emscvt.std\_profiles.tog.30Apr2024” and “10may2024.std\_profiles.xref” to the TCEQ in a format compatible with the SAS point source processing script.

**Table 1. Updated standard VOC profiles by source category.**

VOC Profile Category 1	VOC Profile Category 2	Count
Chemical Reaction	Chemical Manufacturing	7
Chemical Reaction	Petrochemical; Refinery; Catalytic Cracker	1
Chemical Reaction	Pulp And Paper; Reactor	1
Combustion	Basic Oxygen Furnace	1
Combustion	Biomass Burning	1
Combustion	Biomass Burning; Agriculture	4
Combustion	Biomass Burning; Prescribed Fire	4
Combustion	Biomass Burning; Residential Wood Combustion; Fireplace	1
Combustion	Biomass Burning; Residential Wood Combustion; Woodstove	2
Combustion	Biomass Burning; Wildfire	2

VOC Profile Category 1	VOC Profile Category 2	Count
Combustion	Biomass Burning; Wildfire; Prescribed Fire	1
Combustion	Boiler	6
Combustion	Chemical Manufacturing; Flare	1
Combustion	Chemical Manufacturing; Tar Kettle	1
Combustion	Cigarette	1
Combustion	Coke Oven	3
Combustion	Cooking; Charbroiling	1
Combustion	Cooking; Frying	2
Combustion	Electric Generation; Boiler	1
Combustion	Engine	4
Combustion	Flare	1
Combustion	Incinerator	1
Combustion	Industrial; Boiler	1
Combustion	Industrial; Metal; Furnace	2
Combustion	Industrial; Metal; Sintering	1
Combustion	Mineral Products; Rotary Dryer	1
Combustion	Mobile	4
Combustion	Mobile; Aircraft	7
Combustion	Mobile; Marine	1
Combustion	Mobile; Nonroad	1
Combustion	Mobile; Onroad	8
Combustion	Mobile; Onroad; Light Duty	3
Combustion	Oil And Gas; Flare	2
Combustion	Oil And Gas; Well	1
Combustion	Pulp And Paper	3
Combustion	Pulp And Paper; Boiler	1
Combustion	Pulp And Paper; Kiln	1
Combustion	Residential	1
Microbial	Agriculture; Animal	5
Microbial	Agriculture; Food	1
Microbial	Composting	1
Microbial	Landfill	2
Microbial	Wastewater Treatment	1
Miscellaneous	Miscellaneous	44
Volatilization	Chemical Manufacturing	125
Volatilization	Chemical Manufacturing; Fugitives	1
Volatilization	Chemical Manufacturing; Rail Car Or Truck Cleaning	6
Volatilization	Chemical Manufacturing; Spraying	1
Volatilization	Chemical Manufacturing; Tank	4
Volatilization	Consumer Products	11
Volatilization	Degreasing	12
Volatilization	Dry Cleaning	5

VOC Profile Category 1	VOC Profile Category 2	Count
Volatilization	Geogenic	1
Volatilization	Graphic Arts	14
Volatilization	Industrial	5
Volatilization	Industrial; Fugitives	2
Volatilization	Industrial; Metal	4
Volatilization	Industrial; Surface Coating	1
Volatilization	Industrial; Tank	2
Volatilization	Mineral Products	2
Volatilization	Mobile	20
Volatilization	Mobile; Onroad	1
Volatilization	Mobile; Onroad; Light Duty	1
Volatilization	Oil And Gas	1
Volatilization	Oil And Gas; Dehydrator	2
Volatilization	Oil And Gas; Fugitives	3
Volatilization	Oil And Gas; Pond	4
Volatilization	Oil And Gas; Tank	20
Volatilization	Oil And Gas; Transmission	1
Volatilization	Oil And Gas; Well	44
Volatilization	Paint Manufacturing	3
Volatilization	Pesticides	2
Volatilization	Petrochemical	10
Volatilization	Petrochemical; Refinery	7
Volatilization	Petrochemical; Refinery; Cooling Tower	1
Volatilization	Petrochemical; Refinery; Fugitives	3
Volatilization	Petrochemical; Refinery; Tank	2
Volatilization	Petrochemical; Tank	4
Volatilization	Petrochemical; Transport	1
Volatilization	Pulp And Paper	5
Volatilization	Pulp And Paper; Dryer	2
Volatilization	Pulp And Paper; Tank	5
Volatilization	Rubber And Plastics	4
Volatilization	Solvent	44
Volatilization	Surface Coating	32
Volatilization	Surface Coating; Aircraft	1
Volatilization	Surface Coating; Appliances	1
Volatilization	Surface Coating; Architectural	3
Volatilization	Surface Coating; Autos	5
Volatilization	Surface Coating; Can	1
Volatilization	Surface Coating; Marine Paints	1
Volatilization	Surface Coating; Metal Furniture	1
Volatilization	Surface Coating; Oil	1
Volatilization	Surface Coating; Paper	1

VOC Profile Category 1	VOC Profile Category 2	Count
Volatilization	Surface Coating; Rail	1
Volatilization	Surface Coating; Spraying	2
Volatilization	Surface Coating; Traffic Paints	1
Volatilization	Surface Coating; Wood Furniture	1
Volatilization	Surface Coatings	3
Volatilization	Surface Coatings; Aerosol	3
Volatilization	Tank	8
Volatilization	Textile Products	2
Volatilization	Transport	2
Volatilization	Volatile Chemical Products	7
<b>Total</b>		<b>602</b>

### 3.2 Updating the Compound Database

The SAS script uses a compound database with mappings for the CB6 chemical mechanism. We reviewed and updated TCEQ's existing chemical mechanism mappings to include IVOC model species and explicitly map alpha-pinene to the APIN model species. These updates will transition the STARS mapping from CB6 to CB7.

We provided TCEQ with an Excel workbook (TCEQ\_CB7\_IVOC\_Speciation\_Update\_30Apr2024.xlsx) containing updated mappings and notes indicating which mappings were added, modified, or retained as is. Additionally, we supplied the updated CB7 compound database as a text file for use with the SAS script.

## **4 Evaluation of Updated Speciation Data**

The TCEQ integrated the updated standard VOC speciation files into their modeling system and performed emissions processing with EPS3 for a test case for the Houston area (an eight-county HGB area). We reviewed the EPS3 Speciate Emissions (SPCEMS) message files and outputs for the test case to ensure that the updated compound database and standard VOC speciation files are functioning as intended.

Our review revealed substantial differences in point-specific VOC profiles for some sources. Subsequent investigation confirmed that these differences resulted from intentional data updates. These differences occur when a point source has a large portion of unspciated VOC emissions, and the updated standard VOC profile assigned is significantly different from the old profile.

We determined that the changes in point-specific VOC profiles for the HGB test case were reasonable and explained by the data updates developed in this project.

## 5 Conclusions and Recommendations

This project has improved the representation of VOC emissions from Texas point sources in TCEQ's SIP modeling framework. By updating and incorporating new speciation profiles and the chemical mechanism mappings to include IVOC model species and alpha-pinene mapping to APIN, we have improved the accuracy of VOC speciation data used for modeling purposes.

Key updates included enhancing two critical components: (1) speciation profiles that specify the weight fraction of individual VOCs emitted by each source, and (2) the compound database mapping individual VOCs to model species of the CB7 chemical mechanism used by photochemical models like CAMx. We integrated new speciation profiles from the latest SPECIATE (v5.3) database into TCEQ's standard VOC speciation library.

Testing of the updated speciation files for the Houston area (HGB) revealed notable differences in speciation VOC emissions. As such, this project succeeded in improving Texas point source VOC speciation used for SIP modeling.

## 6 References

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