

Prepared for:

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

Prepared by:

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

June 16, 2022

# Update PM Speciation for Texas Point Sources

PREPARED UNDER A CONTRACT FROM THE  
TEXAS COMMISSION ON ENVIRONMENTAL QUALITY

*The preparation of this document was financed through a contract from the State of Texas through the Texas Commission on Environmental Quality.*

*The content, findings, opinions and conclusions are the work of the author(s) and do not necessarily represent findings, opinions or conclusions of the TCEQ.*



**Update PM Speciation for Texas Point Sources  
Final Report**

Ramboll  
7250 Redwood Boulevard  
Suite 105  
Novato, CA 94945  
USA

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

## Contents

<b>Executive Summary</b>	<b>1</b>
<b>1 Introduction</b>	<b>2</b>
1.1 Background	2
1.2 Project Objectives	2
<b>2 Development of Point-Specific Speciation Profiles</b>	<b>3</b>
<b>3 Methodology</b>	<b>4</b>
3.1 Updating EPA PM Speciation Profiles	4
<b>4 Evaluation of Updated Speciation Data</b>	<b>7</b>
<b>5 Conclusions and Recommendations</b>	<b>8</b>
<b>6 References</b>	<b>9</b>

## **EXECUTIVE SUMMARY**

Particulate Matter (PM) leads to regional haze and visibility degradation in protected areas such as National Parks located in Texas. When the Texas Commission on Environmental Quality (TCEQ) conducts air quality modeling for the Texas State Implementation Plan (SIP), it is important to properly characterize PM emissions in regional air quality models which requires applying appropriate chemical speciation profiles to convert total PM emissions present in the inventory to the model species used by air quality models.

This project improved how PM emitted by Texas point sources is represented in the TCEQ's SIP modeling by incorporating new information into TCEQ's emissions processing procedures. We updated two types of data files needed to speciate PM emissions: (1) speciation profiles that specify the weight fraction of individual PM model species relative to the total PM emitted by a source (2) the cross-reference file that assigns speciation profiles to inventory sources. The speciation updates were made by replacing older profiles in TCEQ's standard PM speciation library with new profiles available in the most recent version of the SPECIATE database (v5.1).

# 1 INTRODUCTION

## 1.1 Background

Fine particles ( $PM_{2.5}$ ) are the main cause of reduced visibility (haze) in parts of Texas, including many of our treasured national parks and wilderness areas located in Texas. When the TCEQ conducts air quality modeling for the Texas SIP, it is important to properly characterize PM emissions in regional air quality models which requires applying appropriate chemical speciation profiles to convert total PM emissions present in the inventory to the model species used by air quality models. This step is part of the emissions processing where inventory pollutants are converted into chemical mechanism model species in a step referred to as 'speciation'. As new information becomes available for speciation, the TCEQ's emissions processing procedures need to be updated.

## 1.2 Project Objectives

The purpose of this project is to review and update speciation data for Texas point sources used by the TCEQ to perform PM speciation in SIP modeling.

## **2 DEVELOPMENT OF POINT-SPECIFIC SPECIATION PROFILES**

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

The TCEQ has developed a unique processing methodology that considers each point source individually and retains all reported speciated PM data and, if the speciated data sum to less than total reported PM, characterizes any remaining unreported PM by using EPA speciation profiles (TCEQ, 2003; PES, 2001). The processing approach is implemented in a SAS script along with QA/QC activities such as removing any non-PM species before processing. The resulting point-specific PM 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 PM into model species of the photochemical mechanism.

As new information becomes available for PM speciation, the TCEQ's emissions processing procedures need to be updated. In this project, we reviewed the EPA speciation profiles used by the SAS script to characterize unreported PM emissions and updated these profiles where newer information has become 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 PM speciation profiles. This includes standard EPA PM weight fraction profiles (profiles\_pm2.5.17Mar2015.txt) and corresponding cross-reference file (xref\_pm2.5.05Jun2017.txt). Each of these data inputs and updates are described in detail below.

#### 3.1 Updating EPA PM Speciation Profiles

The unspiciated portion of the PM emissions for each point source is speciated using EPA PM speciation profiles. Each emission point is assigned a default 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 default PM speciation data, we determined that many profiles needed updating to newer profiles available from the most recent version of the SPECIATE database (v5.1; EPA 2020). The SPECIATE profiles can’t be used directly and need to be processed through the Speciation Tool<sup>1</sup> first to calculate the PM model species required by Comprehensive Air Quality Model with Extensions (CAMx). The CAMx format PM profiles from SPECIATE were obtained from a recent Speciation Tool run available on a public GitHub repository<sup>2</sup>. We replaced a total of 90 default PM profiles in TCEQ’s library with 100 new profiles and updated the corresponding cross-reference file based on EPA’s 2016v2 modeling platform<sup>3</sup>. The count of updated PM profiles by source category is shown in Table 1. There is at least one representative profile for each source category shown in Table 1, but some categories have more than one profile to characterize subcategory level details.

**Table 1. New standard EPA PM profiles by source category.**

PM Profile Category 1	PM Profile Category 2	Count
Ash	Industrial	1
Ash	Industrial; Metal	1
Ash	Industrial; Metal; Calciner	1
Ash	Industrial; Metal; Electric Arc Furnace	1
Ash	Industrial; Metal; Furnace; Sintering	1
Atomization	Surface Coating; Spraying	1
Chemical Reaction	Petrochemical; Catalytic Cracker	1
Combustion	Biomass Burning; Agriculture	2
Combustion	Biomass Burning; Prescribed Fire	1
Combustion	Biomass Burning; Prescribed Fire; Slash	1

<sup>1</sup> <https://github.com/CMASCenter/Speciation-Tool>

<sup>2</sup> <https://github.com/CMASCenter/Speciation-Tool/tree/master/outputs>

<sup>3</sup> <https://www.epa.gov/air-emissions-modeling/2016v2-platform>

<b>PM Profile Category 1</b>	<b>PM Profile Category 2</b>	<b>Count</b>
Combustion	Biomass Burning; Residential Wood Combustion; Fireplace; Woodstove	1
Combustion	Biomass Burning; Wildfire	11
Combustion	Boiler	1
Combustion	Boiler; Process Heater; Engine	1
Combustion	Cooking; Charbroiling; Stirfry; Smoke	1
Combustion	Cooking; Frying	2
Combustion	Domestic	1
Combustion	Electric Generation; Boiler	2
Combustion	Industrial; Boiler	2
Combustion	Industrial; Metal; Cupola	1
Combustion	Industrial; Metal; Furnace	2
Combustion	Industrial; Wood Products	1
Combustion	Mineral Products; Furnace	3
Combustion	Mineral Products; Kiln	2
Combustion	Mobile	1
Combustion	Mobile; Aircraft	1
Combustion	Mobile; Marine	1
Combustion	Mobile; Onroad	2
Combustion	Mobile; Onroad; Light Duty; Medium Duty	1
Combustion	Process Heater; Boiler	1
Combustion	Process Heater; Gas Turbine	1
Combustion	Pulp And Paper	1
Combustion	Pulp And Paper; Furnace	1
Combustion	Residential	1
Combustion	Residential; Space Heater And Water Heater	1
Combustion	Waste Combustion	2
Dust	Agriculture	3
Dust	Agriculture; Silo	1
Dust	Chemical Manufacturing	4
Dust	Construction	1
Dust	Geological	3
Dust	Heat Treating	1
Dust	Industrial	2
Dust	Industrial; Metal	4



<b>PM Profile Category 1</b>	<b>PM Profile Category 2</b>	<b>Count</b>
Dust	Industrial; Metal and Construction; Sandblasting	1
Dust	Industrial; Shredding	1
Dust	Industrial; Wood Products	1
Dust	Mineral Products	5
Dust	Mobile; Onroad	2
Dust	Road	2
Miscellaneous	Miscellaneous	4
Volatilization	Chemical Manufacturing	5
Volatilization	Industrial; Metal	2
Volatilization	Mineral Products	1
Volatilization	Petrochemical	1
<b>Total</b>		<b>100</b>

We updated two types of data files that are needed to speciate PM emissions: (1) speciation profiles that specify the weight fraction of individual PM model species relative to the total PM emitted by a source (2) the cross-reference file that assigns speciation profiles to inventory sources. We provided the updated file "profiles\_pm2.5.21Apr2022.txt" and "xref\_pm2.5.21Apr2022.txt" to the TCEQ in a format compatible with the SAS processing script.

## **4 EVALUATION OF UPDATED SPECIATION DATA**

The TCEQ integrated the updated default PM speciation files into their modeling system and performed emissions processing with EPS3 for a test case for the Houston area (HGB). We reviewed the EPS3 Speciate Emissions (SPCEMS) message files and outputs for the test case to ensure that the updated default PM speciation files are functioning as intended. Our review revealed major differences in point-specific PM profiles for some sources although subsequent investigation confirmed that these differences result from intentional data updates. The differences occur when a point source has a large portion of PM emissions that are unspiciated and the assigned updated default PM profile is very different from the old profile. The updated profile can differ from the old profile because of a PM profile update, a cross-reference update, or both. For example, for point sources with SCC 20200201 "ICE Industrial Natural Gas Turbine", the old processing applied profile 92048 "Natural Gas Combustion - Simplified" but the updated processing applied profile 95475 "Composite- Refinery Fuel Gas and Natural Gas Combustion". The two speciation profiles are very different: Profile 92048 has POA of 30% and PEC of 38% whereas profile 95475 has POA of 64% and PEC of 7%. We determined that large changes point-specific PM profiles for the HGB test case were reasonable and are explained by the data updates developed in this project.

## **5 CONCLUSIONS AND RECOMMENDATIONS**

This project improved how PM emitted by Texas point sources are represented in the TCEQ's SIP modeling by incorporating new information into TCEQ's emissions processing procedures. We updated the default EPA speciation profiles that are used to characterize any unspciated portion of PM emissions from each point source in TCEQ's modeling system that creates point-specific speciation profiles. We updated two types of data files needed to speciate PM emissions: (1) speciation profiles that specify the weight fraction of individual PM model species relative to the total PM emitted by a source (2) the cross-reference file that assigns speciation profiles to inventory sources. Testing the updated files for the Houston area revealed differences for some PM emissions from some point sources and subsequent investigation confirmed that these differences were reasonable and explained by the data updates developed in this project. As such, this project succeeded in improving Texas point source PM speciation used for SIP modeling by incorporating new PM speciation profile data.

## 6 REFERENCES

- TCEQ, 2003, "Speciation of Texas Point Source VOC Emissions for Ambient Air Quality Modeling",  
<https://www.tceq.texas.gov/assets/public/implementation/air/rules/stakeholder/hrvoc/2004-02-06/voc-speciation-report.pdf>
- EPA, 2020, "Addendum SPECIATE Version 5.1 Database Development Documentation",  
[https://www.epa.gov/sites/default/files/2020-07/documents/speciate\\_5.1.pdf](https://www.epa.gov/sites/default/files/2020-07/documents/speciate_5.1.pdf)
- Ramboll, 2019, "VOC Speciation Update for Texas Point Sources",  
[https://www.tceq.texas.gov/assets/public/implementation/air/am/contracts/reports/pm/582199237103-20190521-Ramboll\\_VOC\\_Speciation.pdf](https://www.tceq.texas.gov/assets/public/implementation/air/am/contracts/reports/pm/582199237103-20190521-Ramboll_VOC_Speciation.pdf)