

**SPECIATE 4.0 QUALITY MANAGEMENT PLAN (QMP) /
QUALITY ASSURANCE PROJECT PLAN (QAPP)**

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BACKGROUND

SPECIATE is the U.S. Environmental Protection Agency's (EPA) repository of total organic compound (TOC) and particulate matter (PM) speciation profiles of air pollution sources. Among the many uses of speciation data, these source profiles are used to: 1) create speciated emissions inventories for regional haze, particulate matter (PM_{2.5}), and ozone (O₃) air quality modeling; 2) estimate hazardous and toxic air pollutant emissions from total PM and TOC primary emissions; 3) provide input to chemical mass balance (CMB) receptor models; and, 4) verify profiles derived from ambient measurements using multivariate receptor models (e.g., factor analysis and positive matrix factorization).

The selection of sources is a collaborative effort of the SPECIATE Workgroup composed of EPA experts representing each user community for the profiles contained in SPECIATE. Members of the Workgroup have contributed and/or gathered data, and have provided recommendations about which specific speciation profiles were to be included in the EPA SPECIATE database.

The primary purpose of this project is to update the SPECIATE database to capture recent and scientifically-meritorious volatile organic compound (VOC), total organic gas (TOG), and PM speciation profile data available from EPA, state agencies, peer-reviewed literature and other relevant data sources. Another objective of this project was to revise the structure of the SPECIATE database to allow for storage of important information underlying each profile (meta data such as sampling and analysis methods, profile quality ratings, etc.). In addition, supporting data tables were also updated from those in the previous version of SPECIATE. These include the TOG-to-VOC conversion table and the source classification code (SCC) to SPECIATE profile cross-reference table.

This Quality Assurance Project Plan (QAPP) specifies the method by which data to be integrated into the SPECIATE 4.0 database revision are identified for inclusion, rated, and stored. SPECIATE does not involve any laboratory analyses or sampling. Most data are derived (measured, analyzed and inventoried) from those reported by peer-reviewed journal articles, EPA sources, or specific non-EPA expert researchers. All quality assurance (QA) and quality control (QC) performed on the analytical work associated with the data was performed by the primary researchers. SPECIATE provides a storage and management vehicle for the profile data, not a point of origination for profile data, except in the case of composite profiles based on a set of original profiles as described in Section 4 of this document. SPECIATE 4.0 developers made prudent efforts to obtain and evaluate descriptive information about the development of the profiles in order to assess their suitability for inclusion in the SPECIATE 4.0 revision.

TITLE AND APPROVAL SHEET

Program Title SPECIATE 4.0

Lead Organization Office of Research and Development
U.S. Environmental Protection Agency
Research Triangle Park, NC 27711

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Effective Date This Quality Assurance Project Plan (QAPP) is effective from the document date (September 11, 2006) forward.

Contract Numbers EPA Contract Nos. EP-D-06-001, WA 0-03 and 68-D-02-063, WA 4-04

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ACRONYMS AND ABBREVIATIONS

CARB	California Air Resources Board
CMAQ	EPA Models-3 Community Multiscale Air Quality Modeling System
CMB	chemical mass balance
CRPAQS	California Regional Particulate Air Quality Study
DRI	Desert Research Institute
EC	elemental carbon
EPA	U.S. Environmental Protection Agency
HAPs	hazardous air pollutants
NPRI	National Pollutant Release Inventory
O ₃	ozone
OC	organic carbon
PAHs	polycyclic aromatic hydrocarbons
PM	particulate matter
PM _{2.5}	particulate matter with aerodynamic diameter less than or equal to 2.5 micrometers
QA	quality assurance
QAPP	Quality Assurance Project Plan
QC	quality control
RFG	reformulated gasoline
SCC	source classification code
SIP	state implementation plan
TAPs	toxic air pollutants
TCEQ	Texas Commission on Environmental Quality
TOC	total organic compound
TOG	total organic gas
VOC	volatile organic compound
WA	work assignment
WAM	Work Assignment Manager

DISTRIBUTION LIST

A copy of this QAPP, in hardcopy or in electronic format (preferably), is to be received and retained by each person identified below:

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SECTION 1.0 PROJECT OBJECTIVES, ORGANIZATION, AND RESPONSIBILITIES

1.1 Purpose

The SPECIATE user community has a wide range of interests and needs. Receptor modelers use SPECIATE as a source of data for emission source chemical profiles. Photochemical modelers make use of speciation data to properly characterize photochemical reactivity of VOC emissions and the chemical composition of PM emissions. Emission inventory preparers will sometimes turn to SPECIATE to fill data gaps in inventories of toxic air pollutants (TAPs); which include hazardous air pollutants (HAPs) and greenhouse gases (e.g., methane, elemental, or black carbon). Also, control strategy analysts have an interest in the chemical make-up of VOC and PM emissions, so that control programs can better target the appropriate sources. The fundamental requirement of the project is to integrate existing profiles into a central repository for use by the user communities listed above.

1.2 Objectives

A project to update the SPECIATE database began in 2003 under EPA Contract Numbers 68-D-00-265 (work assignments [WAs] 3-28, 4-46, 4-49), and 68-D-02-063, (WAs 2-12 and 4-04).

Work was initiated under WA 3-28 of EPA Contract 68-D-00-265 in October 2003. This work assignment addressed modifications to the design of the database, a protocol for inclusion of future profiles in the revised database, incorporation of profiles into the new database, and suggestions for a user interface to be integrated into the database in the future. This work assignment outlined many additional tasks for future work assignments, including, but not limited to, simplified PM profiles for use with certain models; profile-SCC mappings; and mapping of VOC species to groups for subsequent modeling work.

In August 2004, WA 2-12 under EPA Contract 68-D-02-063 allowed for the incorporation of more profiles into the new SPECIATE database. In December 2004, WA 4-46 under contract 68-D-00-265 included incorporating additional profiles, completing the documentation associated with the database, and developing a protocol for inclusion of profiles obtained from future research projects. In April 2005, WA 4-49 under contract 68-D-00-265 included tasks to complete the SCC-profile assignments, to complete model groupings for both PM and VOC profiles, to complete the database and documentation, and to prepare this QAPP.

In October 2005, WA 0-03 under contract EP-D-06-001 provided for incorporating comments received on draft materials to be incorporated and finalized. In March 2006, WA 4-04 under contract 68-D-02-063 provided for incorporating Canadian data into the SPECIATE database, new profiles as agreed to by the SPECIATE Workgroup, and preparation of the final report.

1.3 Data Requirements

EPA's purpose for the project is to organize and make available all scientifically meritorious VOC and PM speciation profile data from the peer-reviewed literature, and to provide additional meta data elements useful to the users of speciation data, including air quality modelers, source-receptor analysts, and inventory developers.

The logical data model is shown in Figure 1. The design is intended to accommodate the desired modifications and additions to the SPECIATE functionality. The modifications are based on the suggestions from the October 2002 meeting of the SPECIATE Expert Panel held at the American Association for Aerosol Research conference in Charlotte, NC (<http://www.epa.gov/ttn/chief/software/speciate/index.html>), as well as additional recommendations provided by EPA.

The new SPECIATE database is a Microsoft Access relational database containing the following eight tables. Appendix A provides the data dictionary for each of the eight tables.

- The PM_PROFILE table includes, but is not limited to, profile number, name, notes on the profile, and descriptive information about the profile such as, sum of species, test method, and normalization basis. Also included in this table are the ratings, including expert judgment, vintage, data quality, and overall. The use of the ratings is detailed in Section 3 of this document.
- PM_SPECIE table includes the specie identification number, the profile number associated with the specie, the percentage of the specie in the profile, the uncertainty associated with the percentage value, the method used to determine uncertainty, and a description of the analysis method used to determine the specie's percentage in the profile.
- The REFERENCE table includes information that characterizes the reference documents associated with the profiles, including whether or not a particular reference is the primary reference (thus allowing multiple and unlimited references for any profile).
- The GAS_PROFILE table includes, but is not limited to, profile number, name, notes on the profile, and descriptive information about the profile such as, sum of species, test method, and normalization basis. Also included in this table are the ratings, including expert judgment, vintage, data quality, and overall. The use of the ratings is detailed in Section 3 of this document.
- The GAS_SPECIE table includes the specie identification number, the profile number associated with the specie, the percentage of the specie in the profile, the uncertainty associated with the percentage value, the method used to determine uncertainty, and a description of the analysis method used to determine the specie's percentage in the profile.

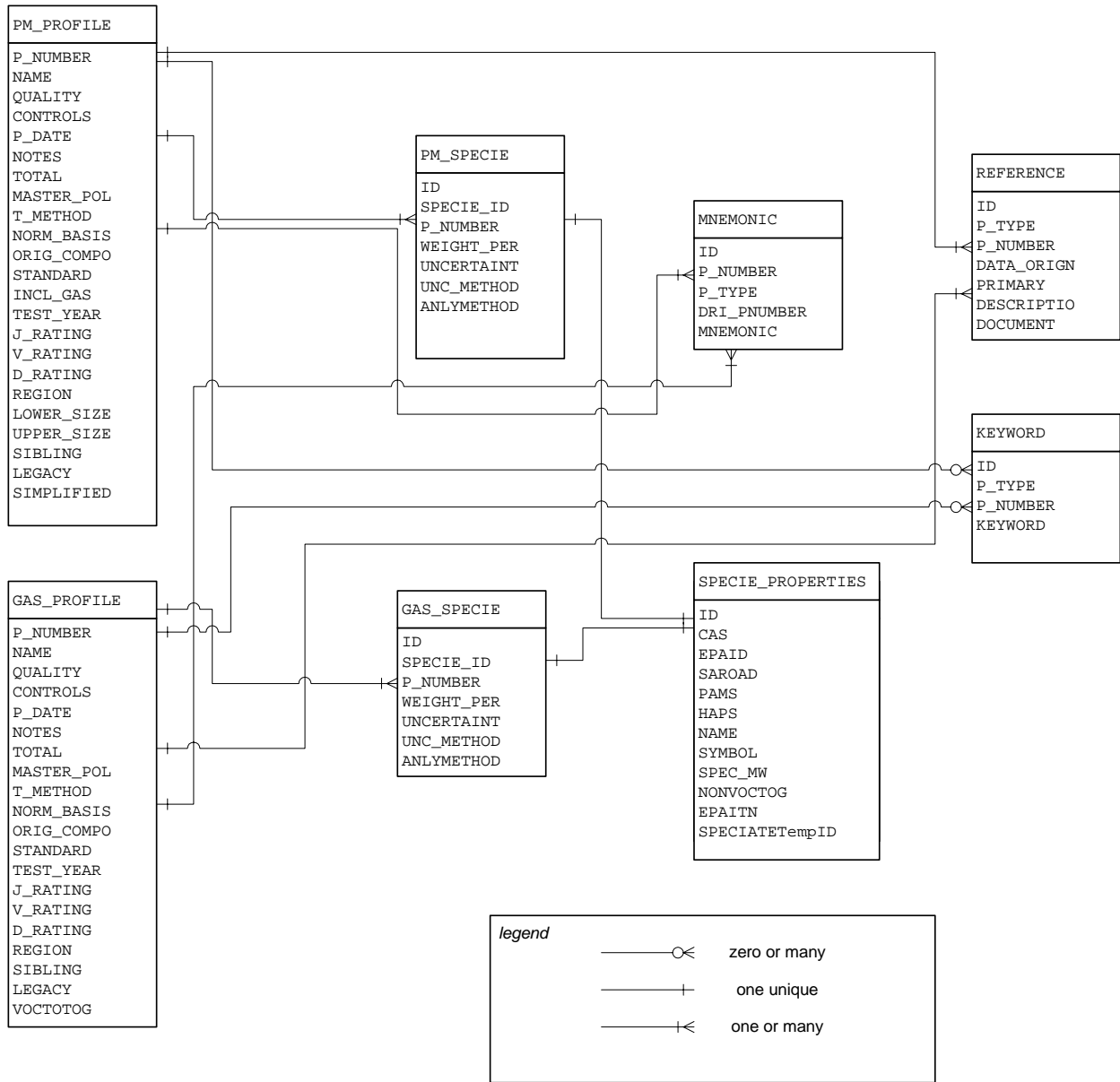


Figure 1. SPECIATE Data Diagram

- The KEYWORD table includes descriptive keywords of profiles. This information can be used in keyword-based searches for profiles.
- The SPECIE_PROPERTIES table includes the identifying numbers associated with the compounds that are species in the database, as well as other characteristic information such as molecular weight.
- The MNEMONIC table includes abbreviated profile names used in CMB receptor models.

It is important to note that SPECIATE is currently a data repository only. No aspect of the user interface may act to influence user's perceptions of the data. In order to present the data to potential users and reviewers that may lack the ability to form queries and reports, the database includes two queries (one each for PM and gas data) that present all of the profile and species information in one large table.

1.4 Disclaimer

Documentation for SPECIATE will include the following disclaimer:

“The records included in the SPECIATE database reflect data that has been collected from publicly available scientific literature and from research organizations. The EPA does not warrant or assume any legal liability or responsibility for the accuracy, completeness, or usefulness of any information, apparatus, product, or process disclosed.”

In addition, a splash screen containing this disclaimer will be added to the SPECIATE database. The splash screen appears as shown in Figure 2 when the user opens the SPECIATE database. The user must click on “Continue”, thus accepting the disclaimer, in order to proceed with using the database. The splash screen disappears when the user selects “Continue”.

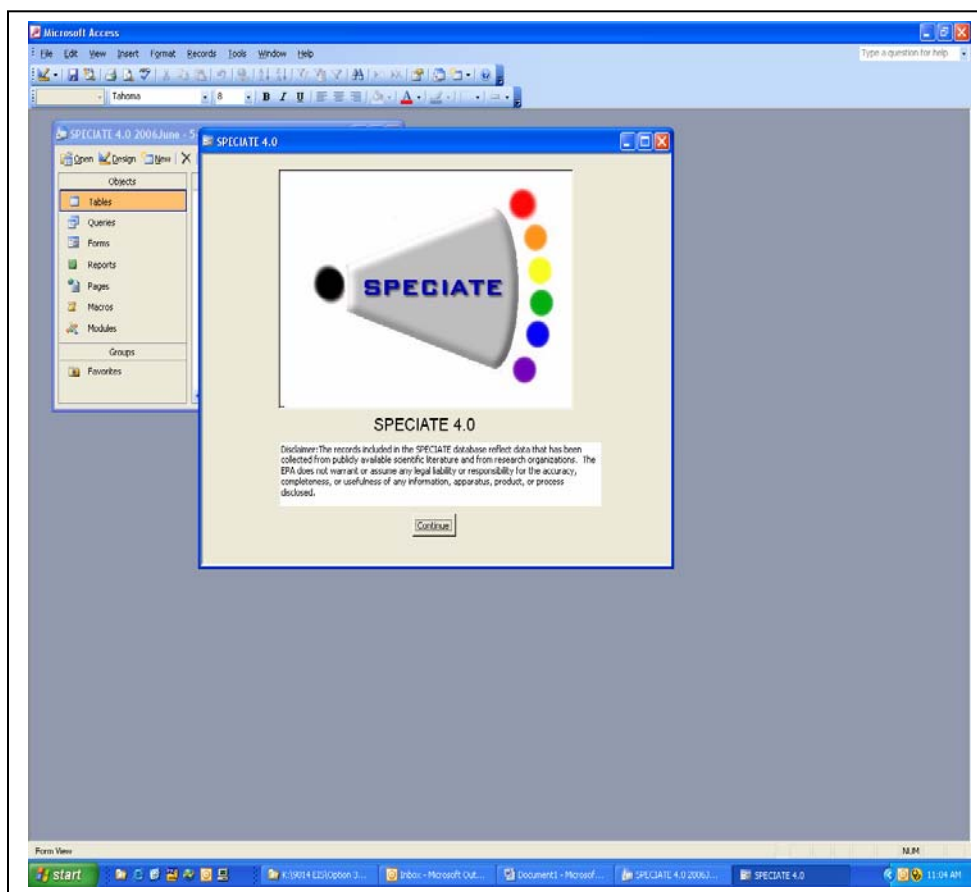


Figure 2. Disclaimer Splash Screen

1.5 Evaluation of Project Objectives

Within the overall goal of providing a comprehensive resource for obtaining speciation profiles, the evaluation of project objectives is a collaborative effort of the SPECIATE Workgroup composed of EPA experts representing each user community for the profiles contained in SPECIATE. The Workgroup discusses and sets objectives through frequent meetings and through group email discussions. The specific members of the Workgroup are identified in the following section; most are career air quality professionals with over 20 years experience in their area of expertise.

1.6 Responsibilities of Participants

The primary contact for the project is Mr. Lee Beck, the Work Assignment Manager (WAM) for the project. SPECIATE efforts are managed by a steering committee coordinated by David Mobley, and staffed by air quality professionals from the EPA. The committee members included:

Richard Baldauf	Marc Houyoux	Tom Pierce
Dennis Beauregard	Bryan Hubbell	George Pouliot
Lee Beck	William L. Johnson	Venkatesh Rao
William Benjey	Larry Jones	Tom Rosendahl
Prakash Bhave	Terry Keating	Bill Russo
Shao-hang Chu	Bill Kuykendal	Ron Ryan
Tom Coulter	Charles W. Lewis	Dave Sanders
Fred Dimmick	Phil Lorang	Golam Sarwar
Shelly Eberly	Deborah Luecken	Joseph Somers
Ron Evans	Douglas McKinney	Bob Stallings
Tyler Fox	David Mobley	Madeleine Strum
Gerry Gipson	Ron Myers	Fred Thompson
Michael Hays	Lucas Neas	Leon Walsh
Tom Helms	Tom Pace	Tim Watkins
James Homolya	Joe Paisie	Jeffrey West

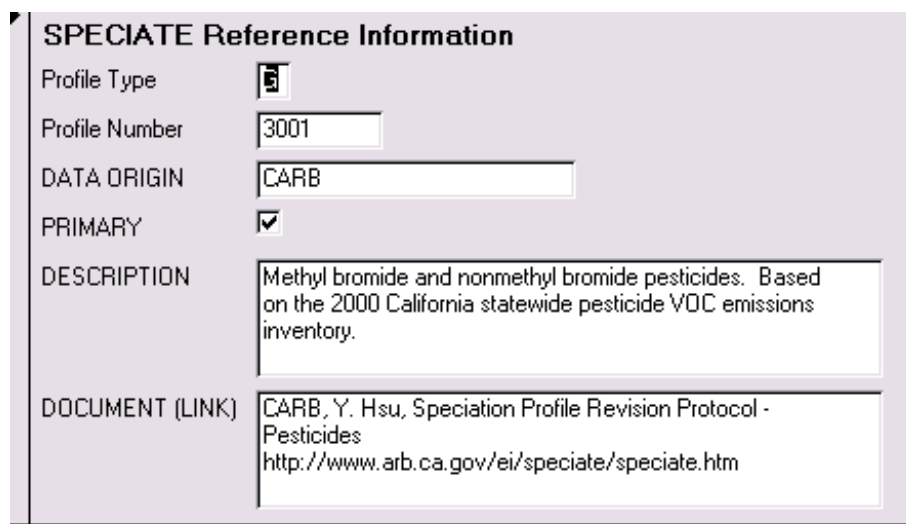
E.H. Pechan & Associates, Inc. maintains a corporate QA/QC policy that requires that all work performed be documented, defensible, of known acceptable quality and consistent with contract requirements. This policy is implemented through an integrated three-tiered approach that includes corporate, department, and project elements. At the corporate level, Pechan management provides oversight of the QA/QC program and approves and enforces the overall program. To assist in implementing these functions, Pechan maintains a corporate QA/QC unit that monitors the program, prepares guidelines, and conducts independent program audits.

Pechan's SPECIATE Project Manager, Mr. Randy Strait, directs all development tasks for the project as directed by and under the guidance of the EPA. Mr. Strait will ensure that all support staff are familiar with and understand the data quality objectives, and the procedures to be followed for meeting the objectives, as well as the requirements of the QA plan.

SECTION 2.0 SOURCES OF SECONDARY DATA

2.1 Specification of Sources

As a repository of secondary data, SPECIATE identifies the source of all data using the REFERENCE table, including fields for data origin, description, and the source documentation itself for every profile. Each profile has one or more records in the REFERENCE table to characterize the references associated with the profile. The sources are specified below in section 2.3. Certain records (composites and simplified profiles) are derived from the gathered profiles. These records are plainly identified and documented; additional information on these records is available in Section 4.1 of this document. A prototype screen from the REFERENCE table is shown in Figure 3.



The screenshot shows a web form titled "SPECIATE Reference Information". It contains several fields: "Profile Type" with a dropdown menu showing "5"; "Profile Number" with a text input field containing "3001"; "DATA ORIGIN" with a text input field containing "CARB"; "PRIMARY" with a checked checkbox; "DESCRIPTION" with a text area containing "Methyl bromide and nonmethyl bromide pesticides. Based on the 2000 California statewide pesticide VOC emissions inventory."; and "DOCUMENT (LINK)" with a text area containing "CARB, Y. Hsu, Speciation Profile Revision Protocol - Pesticides" and the URL "http://www.arb.ca.gov/ei/speciate/speciate.htm".

Profile Type	5
Profile Number	3001
DATA ORIGIN	CARB
PRIMARY	<input checked="" type="checkbox"/>
DESCRIPTION	Methyl bromide and nonmethyl bromide pesticides. Based on the 2000 California statewide pesticide VOC emissions inventory.
DOCUMENT (LINK)	CARB, Y. Hsu, Speciation Profile Revision Protocol - Pesticides http://www.arb.ca.gov/ei/speciate/speciate.htm

Figure 3. Prototype Reference Screen

2.2 Rationale for Selection of Sources

The selection of sources for profiles to be added for SPECIATE 4.0 is a collaborative effort of the SPECIATE Workgroup composed of EPA experts representing each user community for the profiles contained in SPECIATE (see Section 1.5). Profiles are selected for inclusion in SPECIATE based on the Workgroup's perceived need of the candidate profile to address a shortcoming in the existing collection of profiles, or update existing profiles based on improved test/analytical methodologies and/or changes in character of the emission source, taking into account the significance in emissions of the relevant source categories.

Candidate studies that include profiles that might be used in SPECIATE 4.0 are organized and prioritized with input from the SPECIATE Workgroup and the contractor; final action on inclusion of any set of profiles is determined by the SPECIATE Workgroup. Specifically,

Pechan created a spreadsheet to track and prioritize all of the candidate groups of profiles for dissemination and review by the SPECIATE Workgroup.

As detailed in the following section, the process of updating SPECIATE 4.0 with improved profiles entailed soliciting profiles from recognized experts in the field of emissions speciation, including:

- The EPA;
- California Air Resources Board (CARB);
- Desert Research Institute (DRI); and
- Schauer, *et al.*

Then, peer-reviewed journal articles were assessed for potential inclusion in SPECIATE 4.0. The articles and data must:

- Originate from a reputable source;
- Address major source categories;
- Include critical pollutants, such as elemental carbon (EC) and organic carbon (OC);
- Accurately represent the source category with which they are associated; and
- Be the product of a nationally recognized scientist.

The prioritization of the profiles is the work of the collective Workgroup. Specific considerations may include whether the study in question will provide speciation profiles for a category of emissions that are inadequately addressed in the current collection of profiles. The number of profiles included in the study is a quantitative measure that is also considered.

Criteria for exclusion may include:

- Absence of a wide range of species;
- Mass fractions based on engineering judgment, not from source sampling; and
- Absence of certain critical species, such as EC and OC.

Profiles may be added and/or reprioritized based on the proceedings of the Workgroup. The Workgroup operates by consensus; no quantitative record of votes is recorded. Minutes of Workgroup meetings are recorded and available at <http://projects.pechan.com/speciate/Meetings.html>.

The full list of candidate profiles is available at the project website (direct link: <http://projects.pechan.com/speciate/CandidateProfileSetsR2.pdf>). The analysis is summarized in the Summary of Candidate Profiles Memorandum (direct link: <http://projects.pechan.com/speciate/MEMORANDUMCandidateProfilesR2.pdf>).

2.3 Identification of Sources

The source of the data housed in the SPECIATE 4.0 database is fundamental to the use and evaluation of the information by the user community; source information is included with every profile in the database. The SPECIATE 4.0 documentation also identifies the sources of all information included in the database.

Under this project, Pechan reviewed speciation data and profiles obtained from EPA, CARB, DRI, Texas Commission on Environmental Quality (TCEQ), and numerous peer-reviewed journals for inclusion in the new SPECIATE database.

EPA data included the speciation of 155 gasoline and diesel liquid and headspace vapors. Other EPA VOC, TOG and PM data that have been incorporated into the database or are currently being processed include the burning of foliar fuels, agricultural biomass burning, motor vehicle exhaust, pulp and paper boilers, small engines, and iron and steel manufacturing facilities.

CARB assembled many TOG profiles as a result of survey work, testing programs, and other research. These profiles cover consumer products (based on 1997 survey data), aerosol coatings (1997 survey data), architectural coatings (1998 survey data), vehicle hot soak (Hsu, 2003), and other motor vehicle emission sources powered by California reformulated gasoline (RFG).

DRI brought together a large number of area and point source PM speciation profiles from recent studies conducted in several states. TCEQ collected thousands of point source VOC profiles developed as part of the 2000 Texas Air Quality Study. Valuable speciation data are also available in the literature. In particular, the detailed speciation of TOG and PM emissions conducted by Schauer, *et al.* (1998) served as an important source of data for this project. The following sections describe significant datasets from which profiles were obtained.

2.3.1 Environmental Protection Agency Speciation Data

EPA data included the speciation of 374 gasoline and diesel liquids and headspace vapors. Other EPA VOC, TOG, and PM data incorporated into the database include those for the burning of foliar fuels, agricultural biomass burning, motor vehicle exhaust, and iron and steel manufacturing facilities. As of the date of this report, EPA has collected detailed speciation data for:

1. Gasoline and diesel liquids and headspace vapors (Lewis, 2004);
2. Burning of foliar fuels (Hays, *et al.*, 2002), agricultural biomass burning (Hays, *et al.*, 2005);
3. Weyerhaeuser Kraft process recovery boiler at pulp and paper facility (Hays, *et al.*, 2004);
4. Small engines (Beck, 2004); Iron and steel manufacturing facilities (Machemer, 2004);
5. Motor vehicles (Zweidinger, *et al.*, 1990);
6. Oil-fired utility boilers (Beck, 2004);
7. Combustion of residual fuel oil (Huffman, *et al.*, 2000); and

8. Wood-fired industrial boilers (ERG, 2001).

Of the studies mentioned above, speciation data for gasoline and diesel liquids and headspace vapors, burning of foliar fuels and agricultural biomass, iron and steel manufacturing facilities, motor vehicles, combustion of residual oil and wood-fired industrial boilers were processed and incorporated into the new database (items 1,2,5,6, 7, 8 and 9). Other speciation data (items 3 and 4) are still being processed, because they either required more supporting information (e.g., sampling and analytical methods, documentation, number of samples needed for profile quality rating), or the reports were received too late for inclusion.

2.3.2 CASS Group Speciation Data

Schauer, *et al.* (1998) conducted a research study with CARB to characterize seven air pollution sources: meat charbroiling, cooking with seed oils, medium-duty diesel trucks, gasoline-powered motor vehicles, fireplace combustion of wood, cigarette smoke, and industrial spray painting operations. Along with these seven source sectors, this research study also included liquid gasoline and headspace vapor profiles and paved road dust profiles for source receptor modeling. Profiles from five out of the seven source sectors were published in peer-reviewed journals. The other profiles mentioned above were identified in the final report to CARB (Schauer, *et al.*, 1998) and incorporated into the database.

It is important to note that Schauer, *et al.* continued an earlier CARB funded research study by Rogge, *et al.* (1993) that applied several techniques to speciate pollutant compositions. Both studies were Ph.D. dissertations from Dr. Glen Cass's group at the California Institute of Technology. Other speciation profiles by Dr. Cass's research group were also highly recommended by the Workgroup, but have not been incorporated into the database.

Both the Schauer, *et al.* and Rogge, *et al.* studies are extremely detailed in that they speciated hundreds of organic compounds in PM, in addition to ions, metals, EC and OC. These detailed speciation PM profiles are different from most other PM profiles which usually provide EC, OC, ions, and trace element information only. The additional OC speciation data provide important source markers for receptor modeling (e.g., hopanes, steranes, phenols, syringols, and levoglucosan) and TAP emission inventories for health risk assessment (e.g., polycyclic aromatic hydrocarbons (PAHs)).

2.3.3 California Air Resources Board Speciation Profiles

CARB speciation profiles are available to the public on the internet (CARB, 2003). These profiles are used by CARB during the development of state implementation plans (SIP; e.g., to assess photochemical reactivity of VOC mixtures), TAP emission inventories, photochemical modeling, receptor modeling, and other air quality projects. In all, 221 TOG and 3 PM profiles from CARB were selected for incorporation into the new SPECIATE database. These profiles cover emission sources such as consumer products, aerosol coatings, architectural coatings, pesticides, landfill gas, wastewater treatment plants, thinning solvent-mineral spirits, degreasing solvents, vehicle hot soak, and other motor vehicle sources. Other CARB profiles exist in the

previous SPECIATE 3.2 database. Additional profiles were developed as part of CARB funded projects to DRI, and these profiles are included under the DRI data discussion below.

2.3.4 Desert Research Institute Speciation Profiles

In total, 1,182 PM speciation profiles were obtained from DRI and incorporated into the database. The source sectors represented emissions from geological material soils, vegetative burning, industrial fuel combustion, forest fires, road dust, refineries, coal combustion, motor vehicles, and many others. DRI prepared an additional set of profiles from the Lake Tahoe Source Characterization Study (Kuhns, 2004), and a study on middle- and neighborhood-scale variations of PM₁₀ source contributions in Las Vegas, Nevada (Chow, *et al.*, 1999). These PM profiles will be incorporated into a later version of SPECIATE.

DRI was to provide profiles for the Gasoline-Diesel PM Split Study (Clark, *et al.*, 2002) and the California Regional Particulate Air Quality Study (CRPAQS). However, these studies were not completed by the time the WA ended under which DRI was to provide profiles from these studies. The data from the Gasoline-Diesel PM Split Study is now available on Department of Energy, National Renewable Energy Laboratory (NREL) web site. The profiles will be included in SPECIATE Version 4.1 as allowed by the WA budget.

2.3.5 Texas Commission on Environmental Quality Speciation Profiles

Speciation data from the report *Speciation of Texas Point Source VOC Emissions for Ambient Air Quality Modeling* (Cantu, 2003) were downloaded and reviewed for inclusion in the SPECIATE 4.0 database. The TCEQ VOC profile database contains 9,447 VOC speciation profiles, which are associated with the Texas 2000 Air Quality Study (PES, 2003). Along with the profiles, this database includes a cross-reference table to link emission source identification numbers for each facility to the VOC speciation profiles. These point source profiles were derived from annual speciated VOC emissions reported by emitting facilities in Texas. Other Texas area source VOC profiles are essentially EPA SPECIATE profiles. The Workgroup recommended including 5 refinery and 3 olefin manufacturing plant profiles (Allen, 2004) into the database. However, these profiles will be given a low quality rating because meta data (e.g., analytical and sampling methods, source documentation, number of samples needed for profile quality rating) is not readily available and significant resources would be required to retrieve the underlying information (i.e., reviewing the facility reports, likely maintained at the facilities) to develop the meta data.

2.3.6 Additional Profiles for Potential Inclusion

More than 800 peer-reviewed journal articles and technical reports were identified in the literature for consideration. Pechan prepared a detailed analysis of available profile datasets that were not included in SPECIATE 3.2. This analysis includes the number and type of profiles available in each study as well as the priority and level of effort required to integrate the profiles (see Section 2.2 above).

2.3.7 Canadian-specific Speciation Profiles

Pechan will search for emission profile-related data specific to Canadian emission sources. A prime source of this data is expected to be Environment Canada's National Pollutant Release Inventory (NPRI). One of the requirements of the NPRI is that emitters of VOCs in certain categories are required to perform stack-specific speciated VOC reporting. The resultant data must be in speciated format. Consequently, the data reported to the NPRI is likely to be compatible with the SPECIATE database. Pechan will examine the NPRI database to determine the applicability of data for inclusion into SPECIATE, and then incorporate that data into SPECIATE. Pechan will also perform a literature search to seek out other published sources of speciated emissions data that are specific to sources located in Canada. Unpublished sources of Canadian data such as electronic databases will also be considered for inclusion into SPECIATE. Pechan will coordinate with the Workgroup and Environment Canada in deciding on what data to use for developing profiles for addition to the SPECIATE database. In all cases, data sources will be fully referenced and annotated with any comments to allow users to determine data applicability and accuracy.

SECTION 3.0 QUALITY OF SECONDARY DATA

3.1 Quality Requirements of Secondary Data

Data housed in SPECIATE 4.0 must originate from one of the following sources:

- Peer-reviewed data appearing in journal articles;
- Products of other EPA projects; or
- A select group of expert scientists in consultation to the EPA.

The method of identifying data for inclusion used by the SPECIATE Workgroup is discussed in Section 2.2. A quality rating that captures specific quantitative aspects of the data included in each profile is described in the next section.

Candidate data must include the analysis method used to determine the weight percent of each specie, as well as the uncertainty of the stated weight percentage and the method used to calculate uncertainty.

3.2 SPECIATE 3.2 Legacy Profiles

The profiles in SPECIATE 3.2 have been incorporated into the SPECIATE 4.0 database. The GAS_PROFILE and PM_PROFILE tables in the SPECIATE 4.0 database both contain a field named “LEGACY” to identify profiles that originate from SPECIATE 3.2 (see Table 1 for the definition of this field). SPECIATE 3.2 records are clearly discernable by the yes/no criterion for this field (“yes” identifies a SPECIATE 3.2 profile). The data from SPECIATE 3.2 are reformatted for storage in the new SPECIATE database, but the additional fields that appear in SPECIATE 4.0 that do not appear in SPECIATE 3.2 are not populated. The SPECIATE 3.2 profiles are not subject to the SPECIATE 4.0 profile rating criteria discussed in the next section.

3.3 Profile Rating Criteria

SPECIATE is a legacy application that the EPA and other environmental stakeholders have used for many years. This SPECIATE update project is intended to add profiles to the SPECIATE database based on recent research and efforts as described in Section 2. Rating criteria were established for the profiles to be added to the database and are described in the following paragraphs.

The profile ratings that were developed for the newly added source profiles are based on the following criteria:

- *V-rating (profile vintage)* is based on the vintage of the profile which reflects measurement technology and methodology. For profiles before Year 1980 – score = 1, 1980-1990 score = 2, 1991-1995 score = 3, 1996-2000 score = 4 and after Year

2000 score = 5. These data are housed in the V_RATING field in the PM and gas profile tables.

- *D-rating (number of samples)* is given a “1” (poor) to “4” (excellent) rating. This category is rated based on the number of samples: # of samples > 10 score = 4; 5-9 samples score = 3; 3-4 and composite samples score = 2; 1-2 or unknown # of samples score = 1. These data are housed in the D_RATING field in the PM and gas profile tables.
- *Quality Score* = (V-rating) x (D-rating). This rating is found in the PM and/or gas profile tables under the field names QUALITY, V_RATING, and D_RATING, respectively. As discussed above, SPECIATE 3.2 profiles will not have entries for V_RATING or D_RATING (or J_RATING shown below), however, they retain their legacy quality rating expressed numerically (5 = A, 1=E). This convention readily distinguishes any numeric value in the QUALITY field as a hold-over from SPECIATE 3.2. EPA SPECIATE 3.2 Documentation does not identify how the quality ratings were selected.

Profile quality is rated from A (excellent) to E (poor) as shown in Table 1.

Table 1. Overall Profile Quality Ratings

Profile Quality	<i>Quality Score Ranges</i>
A	17-20
B	13-16
C	9-12
D	5-8
E	<5

- *J-rating (expert judgment)* is given a “1” (poor) to “5” (excellent) rating. This value is based on the information underlying each profile including, but not limited to:
 - Profile composition;
 - Relative ratios of species within the profile;
 - Sum of the speciated mass fractions; and
 - Supporting documentation.

Due to complications of each profile, we were unable to develop an objective rule by which to assign the rating. These inherently qualitative values are assigned by the principal investigator for profiles obtained from DRI or by Pechan technical staff otherwise per the guidance of the SPECIATE Workgroup. The Workgroup reviewed the proposed work product. DRI and Pechan have extensive experience in source testing for speciation and processing speciated data for emissions inventories, toxic emissions assessment, photochemical modeling, and source-receptor modeling. The technical staff has published numerous peer-reviewed papers, prepared speciation profiles and methodologies for air quality management agencies. Owing to the subjective nature of this rating, it is not a component of the Overall Profile Quality Rating. The

overall quality rating and its constituent ratings, as well as the expert judgment rating, are available to the user and auditor for their consideration. Users may consider the ratings as well as the reference and summary information about the profiles housed in the profile tables to determine the suitability of a profile to their needs.

SECTION 4.0 DATA REPORTING, DATA REDUCTION, AND DATA VALIDATION

4.1 Data Reduction Procedures

COMPOSITE PROFILES

Many large emission source categories, such as agricultural burning and paved road dust, have multiple speciation profiles in the SPECIATE 4.0 database. The Workgroup prepared 47 composite PM profiles and then added them to the database.

Users may employ the composite profiles to avoid manual comparison of several relevant but diverse profiles, using the composites as an indication of central tendency for the source category. Users may equally prefer their own analysis of the constituent profiles, determining the best fit for their needs, thereby obviating the need for the composites.

The PM-composite profiles are identified by P_NUMBER's that start with "91xxx". The term "composite" is also included at the end of the name in the "NAME" field in the PM_PROFILE table. The composite profiles are easily identified by the ORIG_COMPO field (allowed value = "O" for Original, "C" for Composite, Null for legacy profiles). The "NOTES" field in the PM_PROFILE table identifies the individual profiles (included in the SPECIATE database) upon which the composite profiles are based. The documentation provided in the "NOTES" field is also provided in the "DESCRIPTIO" field in the REFERENCE table; the "DOCUMENT" field in the REFERENCE table is null since the composite profiles are based on more than one individual profile. Users may look-up the references for the individual profiles in the database to identify the references supporting the PM-composite profiles.

PM-SIMPLIFIED PROFILES

PM-simplified profiles are those based on full PM profiles collapsed to five species: Elemental Carbon, Organic Carbon, Sulfate, Nitrate, and PMOther (remaining mass fraction representing all other species). The Workgroup prepared 95 simplified PM profiles and then added them to the database. PM-simplified profiles are employed in air quality models (e.g., CMAQ) that use the simplified, five-species approach. For the composite profiles prepared for SPECIATE 4.0, simplified profiles were prepared after the composite profiles were introduced into the database. The PM-simplified profiles are identified by P_NUMBER's that start with "92xxx". The PM-simplified profiles are also identified by a symbol in the "SIMPLIFIED" field in the PM_PROFILE table.

4.2 Data Validation Procedures

A Candidate Release version of the SPECIATE documentation and database is released to the SPECIATE Workgroup prior to final delivery of the products. The Workgroup reviews the content of the database and documentation, referring comments to the contractor via the WAM.

For documentation, the review may include detailed reading, checking of references, and checking of consistency. For the database, review may include detailed review of certain profiles with which the reviewer has experience, and/or database queries and manipulation of the data to assess its suitability in particular processing models. Received comments may be documented in the minutes of Workgroup meetings and in email records. The contractor integrates the comments, resolving any potential conflicts among comments by working with the members of the SPECIATE Workgroup and the WAM. The SPECIATE Project Website is used to record findings and to document comments and issue resolution. Issues are documented via technical memoranda posted in the documentation section. A web-based discussion forum is also available.

The legacy SPECIATE 3.2 data are offered as-is to accommodate previous users of these profiles, except for profiles that contained errors identified by the Workgroup. For profiles that contained errors, the profiles were revised based on the original data sources or the Workgroup's recommendations.

4.3 Deliverable Products

Deliverable products include a Final Report based on the activities conducted in these work assignments that make up the SPECIATE project. The Final Report includes sections on the database structure, the profiles in the database, issue-specific notes and comments on the data and its quality, source profile preparation methods, and references.

The SPECIATE database prepared under this project will be delivered in Microsoft Access format, including one or more methods of viewing the SPECIATE data that do not require programming skills. This project does not currently include the development of a user interface; rather, the database will be the repository for speciation profiles and related information.

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APPENDIX A. DATA DICTIONARY

Table A-1. Descriptive Data Dictionary

	Field	Type¹	Length²	Decimals	Description
	PM_PROFILE Table				
Primary key	P_NUMBER	C	10		PM Profile Number
	NAME	C	255		PM Profile Name
	QUALITY	C	3		Quality rating (A-E) of the profile (related to the products of the V and D ratings, see next report section for an explanation)
	CONTROLS	C	100		Emission Controls Description
	P_DATE	D			Date profile added
	NOTES	M			Notes
	TOTAL	N	6	2	Sum of species percentages for a given profile, excluding organic species, inorganic gases, and elemental sulfur in individual PM profiles. (See Section IV.F "Double Counting Compounds" of this report for rationale.)
	MASTER_POL	C	5		Indicates the pollutant to be used in calculation. Allowed value: 'PM' In the future, other values may be allowed (e.g., PM_PRI, PM_FIL, PM_CON)
	T_METHOD	M			Description of sampling method
	NORM_BASIS	C	25		Description of how profile was normalized (see section IV.E for details)
	ORIG_COMPO	C	1		Specifies whether the profile is original or composite. Allowed values: 'C', 'O'
	STANDARD	L	1		Indicates whether the profile is provided by EPA SPECIATE (standard) or user-added. The database is constructed to allow users to add profiles.
	INCL_GAS	L	1		Indicates whether or not the profile includes inorganic gas species (e.g., sulfur dioxide, hydrogen sulfide, oxides of nitrogen, etc.)
	TEST_YEAR	N	4	0	Indicates year testing was conducted
	J_RATING	N	4	2	Subjective expert judgment rating based on general merit (see section II.D for an explanation)
	V_RATING	N	4	2	Vintage based on TEST_YEAR field (see section II.D for an explanation)
	D_RATING	N	4	2	Data quality rating based on number of observations, robustness (see section II.D for an explanation)
	REGION	C	50		Geographic region of applicability
	LOWER_SIZE	N	5	2	Identifies lower end of aerodynamic diameter particle size, micrometers
	UPPER_SIZE	N	5	2	Identifies upper end of aerodynamic diameter particle size, micrometers

Table A-1 (continued)

	Field	Type¹	Length²	Decimals	Description
Foreign key	SIBLING	C	10		GAS Profile number; samples taken from the same source and study, if available.
	LEGACY	L	1		Was the profile taken from SPECIATE 3.2?
	SIMPLIFIED	L	1		Is the profile a PM Simplified Profile?
PM_SPECIE Table					
Primary key	ID	N	9	0	Unique Identifier
Foreign key	SPECIE_ID	N	9	0	Specie Identifier (The same as ID in SPECIE_PROPERTIES)
Foreign key	P_NUMBER	C	10		PM Profile number (Link to PM_Profile Table)
	WEIGHT_PER	N	7	3	Weight percent of pollutant (%)
	UNCERTAINT	N	7	3	Uncertainty percent of pollutant
	UNC_METHOD	C	25		Description of method used to calculate uncertainty
	ANLYMETHOD	C	50		Description of Analytical method (e.g., X-ray fluorescence spectroscopy, ion chromatography, etc.)
REFERENCE Table					
Primary key	ID	N	9	0	Unique Identifier
Foreign key	P_TYPE	C	1		Indicates PM or GAS. Allowed values: P (PM), G (Gas)
Foreign key	P_NUMBER	C	10		Profile number (Link to PM_PROFILE and GAS_PROFILE tables)
	DATA_ORIGN	C	50		Source of data (e.g., EPA APPCD, Schauer, CARB, DRI, Literature, etc.)
	PRIMARY	L			Designates a reference as primary. When a profile is based on multiple references, this field allows one reference to be tagged as the primary reference.
	DESCRIPTIO	M			Stores the descriptive information about the profile.
	DOCUMENT	M			Complete reference citation.
GAS_PROFILE Table					
Primary key	P_NUMBER	C	10		GAS Profile Number
	NAME	C	255		GAS Profile Name
	QUALITY	C	3		Quality rating (A-E) of the profile (related to the products of the V and D ratings, see section II.D for an explanation)
	CONTROLS	C	100		Emission Controls Description
	P_DATE	D			Date profile added
	NOTES	M			Notes

Table A-1 (continued)

	Field	Type¹	Length²	Decimals	Description
	TOTAL	N	6	2	Sum of organic gas species percentages for a given profile
	MASTER_POL	C	4		Indicates the pollutant to be used in calculation. Allowed values: 'VOC', 'TOG'. When methane was not measured in a study, ethane, acetone and other non-VOCs are removed from the profile and it is defined as a VOC profile.
	T_METHOD	M			Description of sampling method
	NORM_BASIS	C	25		Description of how profile was normalized
	ORIG_COMPO	C	1		Specifies whether the profile is original or composite. Allowed values: 'C','O'
	STANDARD	L	1		Indicates whether the profile is provided by EPA SPECIATE (standard) or user-added. The database is constructed to allow users to add profiles.
	TEST_YEAR	N	4		Indicates year testing was conducted
	J_RATING	N	4	2	Subjective expert judgment rating based on general merit (see section II.D for an explanation)
	V_RATING	N	4	2	Vintage based on TEST_YEAR field (see section II.D for an explanation)
	D_RATING	N	4	2	Data quality rating based on number of observations, robustness (see section II.D for an explanation)
	REGION	C	50		Geographic region of source
Foreign key	SIBLING	C	10		PM Profile number; samples taken from the same source and study, if available.
	LEGACY	L	1		Was the profile taken from SPECIATE 3.2?
	VOctoTOG	N	7	3	VOC to TOG conversion factor
GAS_SPECIE Table					
Primary key	ID	N	9	0	Unique Identifier
Foreign key	SPECIE_ID	N	9	0	Species Identifier (Must be the same as ID in SPECIE_PROPERTIES)
Foreign key	P_NUMBER	C	10		GAS Profile Number (Link to GAS_PROFILE table)
	WEIGHT_PER	N	6	2	Weight percent of pollutant (%)
	UNCERTAINT	N	7	3	Uncertainty percent of pollutant
	UNC_METHOD	C	25		Description of method used to calculate uncertainty
	ANLYMETHOD	C	50		Description of Analytical method (e.g., GC/FID, GC/MS, HPLC/UV, etc.)

Table A-1 (continued)

	Field	Type¹	Length²	Decimals	Description
KEYWORD Table					
Primary key	ID	N	9	0	Unique Identifier
Foreign key	P_TYPE	C	1		Indicates PM or GAS. Allowed values: P, G
Foreign key	P_NUMBER	C	10		Profile Number (Link to PM_PROFILE and GAS_PROFILE Tables)
	KEYWORD	C	255		Keyword describing profile
SPECIE_PROPERTIES Table					
Primary key	ID	N	9	0	Unique Identifier (Link to PM_SPECIES and GAS_SPECIES tables)
	CAS	C	50		Chemical Abstract Service number assigned to pollutant (with hyphens) (blank if no CAS)
	EPA_ID	C	50		EPA Chemical Identifier; to be provided by EPA Substance Registry System for species without CAS numbers
	SAROAD	C	5		Storage and Retrieval of Aerometric Data (SAROAD) code
	PAMS	L	1		Is PAMS pollutant? (Yes or No)
	HAPS	L	1		Is Hazardous Air Pollutant? (Yes or No)
	NAME	C	255		Pollutant name
	SYMBOL	C	9		Standard chemical abbreviation (provided by Eric Fujita, DRI)
	SPEC_MW	N	6	2	Species molecular weight
	NonVOCTOG	L	1		Is this species not regarded as a volatile organic gas?
	EPAITN	C	9		EPA Internal Tracking Number
	SPECIATETempID	C	25		SPECIATE Temporary ID
MNEMONIC Table					
Primary key	ID	N	9	0	Unique Identifier
Foreign key	P_TYPE	C	1		Indicates PM or GAS. Allowed values: P (PM), G (Gas)
Foreign key	P_NUMBER	C	10		Profile number (Link to PM_PROFILE and GAS_PROFILE tables)
	DRI_PNUMBR	C	6		DRI profile number (Original DRI profile numbers)
	MNEMONIC	C	60		Alphanumeric code unique to each profile. Used in CMB input files.

¹ Field types. C: Character; D: Date; L: Logical; M: Memo; N: Numeric; Object.

² Length – length allowed.