Speciation Tool User's Guide

Version 4.0

DRAFT

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1.0 BACKGROUND

Air Quality Models (AQM) contain a set of equations that use representative lumped modeling compounds to simulate complex atmospheric chemistry. The emission inventory, an important input to the AQM, consists of components such as CO, NOx, total volatile organic compounds (VOCs), and particulate matter (PM). The emission inventory components, also known as pollutants, must be converted to the lumped modeling compounds for air quality modeling.

The Speciation Tool is a stand-alone tool that was developed to generate the factors needed to convert the emission inventory components to the AQM lumped modeling compounds. The conversion process is referred to as *'speciation'*. The factors are referred to as '*split factors'*; i.e. we 'split' total VOCs to olefins, aldehydes, etc. The '*chemical mechanism*' is the mapping of the emission inventory pollutants to the AQM compounds.

In the past, most Air Quality Modeling was performed based solely on criteria air pollutants (CAPS). However, more frequently, the trend is to develop inventories that include both criteria and toxic air pollutants. Toxic air pollutants, also known as hazardous air pollutants (HAPS) are known or suspected to cause serious health effects. The Speciation Tool supports the availability of both CAPS and HAPS. It was designed to either integrate the HAPS in the chemical mechanism or not and to include both active and tracer species in modeling.

The Speciation Tool supports chemical mechanisms for both VOCs and PMs.

2.0 INTRODUCTION

This document provides a User's Guide for running the Speciation Tool version 4.0. The purpose of the Speciation Tool is to generate the chemical speciation profiles required by emissions processors to convert emission inventory compounds to air quality modeling compounds.

The Speciation Tool supports speciation profile entries for VOC compounds and particulate matter less than 2.5 microns ($PM_{2.5}$) based on EPA's SPECIATE 4.5 profile assignments. The VOC chemical mechanisms included in the Speciation Tool are carbon bond mechanism versions 4, 5, and 6 (CBIV, CB05, CB6) and the 1999 and 2007 Statewide Air Pollution Research Center mechanism (SAPRC99, SAPRC99B, SAPRC07, and SAPRC07T). The $PM_{2.5}$ mechanisms included are the CMAQ version 5 (AE5) and version 6 (AE6) aerosol mechanisms.

The Speciation Tool also produces the factors needed to convert VOC mass to Total Organic Gases (TOG) mass; this is the VOC-to-TOG conversion factor. These factors are needed when an emission inventory is reported as VOC which is often the case. Since the gas profiles are computed based on TOG and the inventory is reported as VOC the VOC-to-TOG conversion factor is applied to the inventory VOC to estimate TOG. The speciation profiles are then applied to the TOG value with no loss of mass.

The output files of the Speciation Tool are intended to be used in the Sparse Matrix Operator Kernel Emissions (SMOKE) Model. These are the SMOKE speciation profile file (GSPRO) and pollutant-to-pollutant conversion file (GSCNV). The GSCNV file generated by the Speciation Tool is formatted for SMOKE version 2.3 and higher and will not work for earlier versions of the software. The Speciation Tool does not create the SMOKE speciation cross-reference file (GSREF); you must ensure the speciation profile codes output by this tool correspond to the codes assigned to emissions sources by the SMOKE GSREF file.

The Speciation Tool is a PostgreSQL database application with a Perl script interface. It is designed for concurrent multiple user access where each run has a unique user specified name. The Speciation Tool assigns the run name to a database schema for storing temporary tables and results. As a database convention, a schema is essentially a container that stores tables and functions in a selected database. Think of a schema as a folder in the Speciation Tool database. The *shared* schema in the Speciation Tool database, created during initialization, holds the imported data of the mechanism definitions, profile descriptions, profile definitions, and species properties. It also retains the functions which compute the speciation split factors. Before running the Speciation Tool, PostgresSQL, Perl, and Perl libraries must be installed. Speciation Tool scripts must be run to confirm the correct installation of these ancillary tools and to initialize the database. A successful initialization will create the database, load the tool functions, create the *shared* schema with defined tables, and import default data files to the *shared* schema. The instructions for these tasks are provided in Chapter 3.

Chapter 4, Running the Speciation Tool, provides the details for running the model; run parameters and options are described. A Speciation Tool run creates a named schema in the

Speciation Tool database. Refer to the Exhibit 2-1 below; initialization creates the *sptoolv4_0* PostgreSQL database with schema *shared* and each run will create an additional named schema based on the user specs. In this example two runs have been made; cb05_criteria and saprc_toxics. Chapter 5, Applications and Methodology, provides additional details of the Speciation Tool calculations. Chapter 6, FAQ, addresses both basic and advanced questions on using the Speciation Tool model.

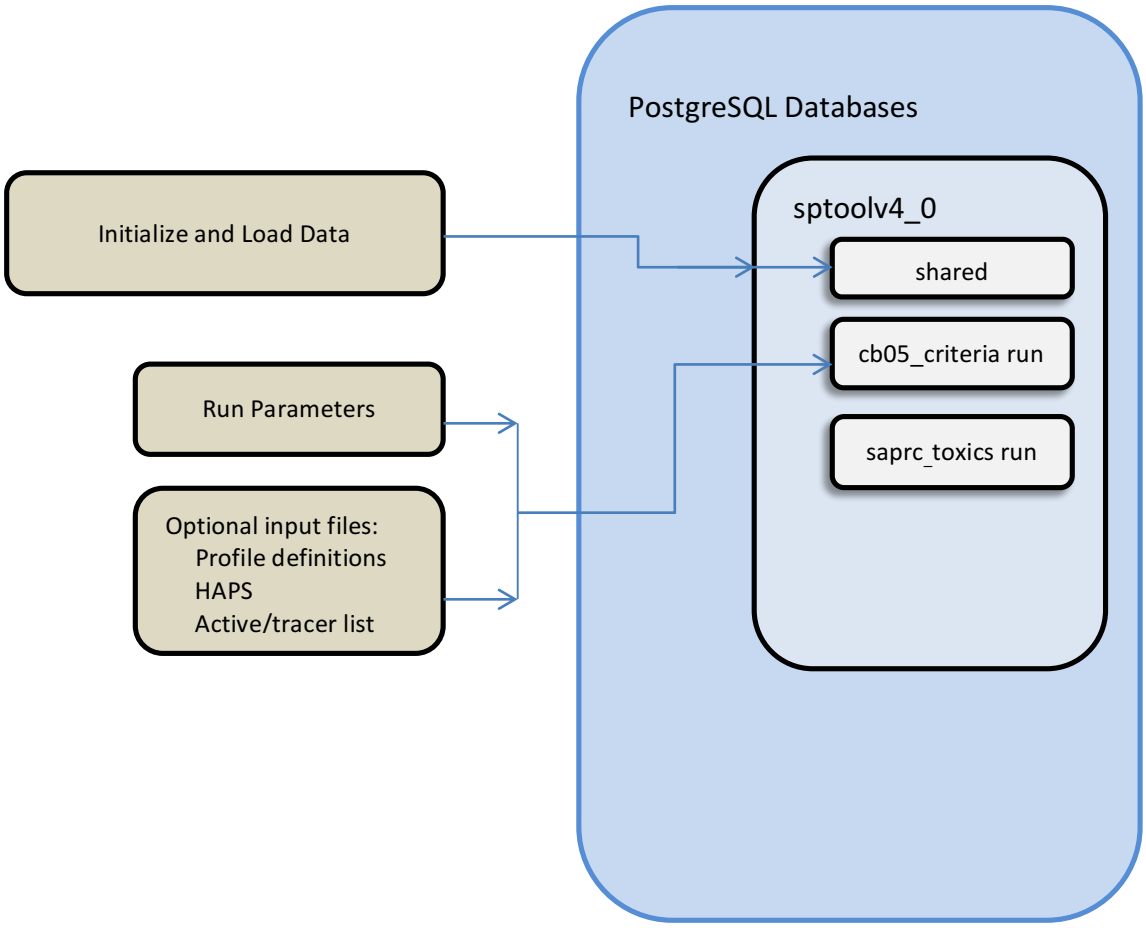


Exhibit 2-1. Speciation Tool Initialization and Run schemas.

3.0 INITIALIZE THE SPECIATION TOOL DATABASE

The Speciation Tool is written in PostgreSQL using the Perl Database Interface (DBI) and CSV parser (Text::CSV). These software products are open source and available on the internet. You must install PostgreSQL and Perl prior to running the Speciation Tool. Appendix A has instructions for installing these packages and options required.

The Speciation Tool must be initialized prior to making any runs. Initialization steps include:

- Get the Speciation Tool package
- Extract files
- Set the home directory
- Run the initialization script

Following is a detailed description of each of these steps. In addition, a quick step-by-step approach is provided for those already familiar with software setup and database applications.

3.1 Quick Start

For a quick start follow these steps. The details of each of these steps are provided in the following sections.

1. Create a Speciation Tool directory

2. Extract the Speciation Tool installation files.
    a. Change to the Speciation Tool directory.
    b. Copy the Speciation Tool package to this directory.
    c. Extract and uncompress the zipped file.

3. Verify required software packages are available. See Appendix A for software packages.
    a. Run *./spool_reqd_checks.sh*

4. Set environment variables.
    a. Edit *Assigns.sptool*; set SPTOOL_HOME.
    b. source Assigns.sptool

5. Initialize the Speciation Tool database.
    a. Execute *./init_sptooldb_v4.0.csh*

6. Execute the provided test case.
    a. Change to the run directory; cd /run
    b. Run *./cb05_notoxics.job*

7. Review and compare results.
    a. Change to output directory; cd ../output
    b. Compare results to provided test case files.

3.2 Install Speciation Tool

To install the Speciation Tool, create a Speciation Tool home directory from which to work. In the example below it is */sptool* but you can specify any valid directory name. Copy the installation package file *sptoolv4_0_May2013.gztar* to the directory and extract the Speciation Tool files:

```
> tar   -xvzf    sptoolv4_0_May2013.gztar
```

After the extraction you should see the files and directories listed in Exhibit 3-1.

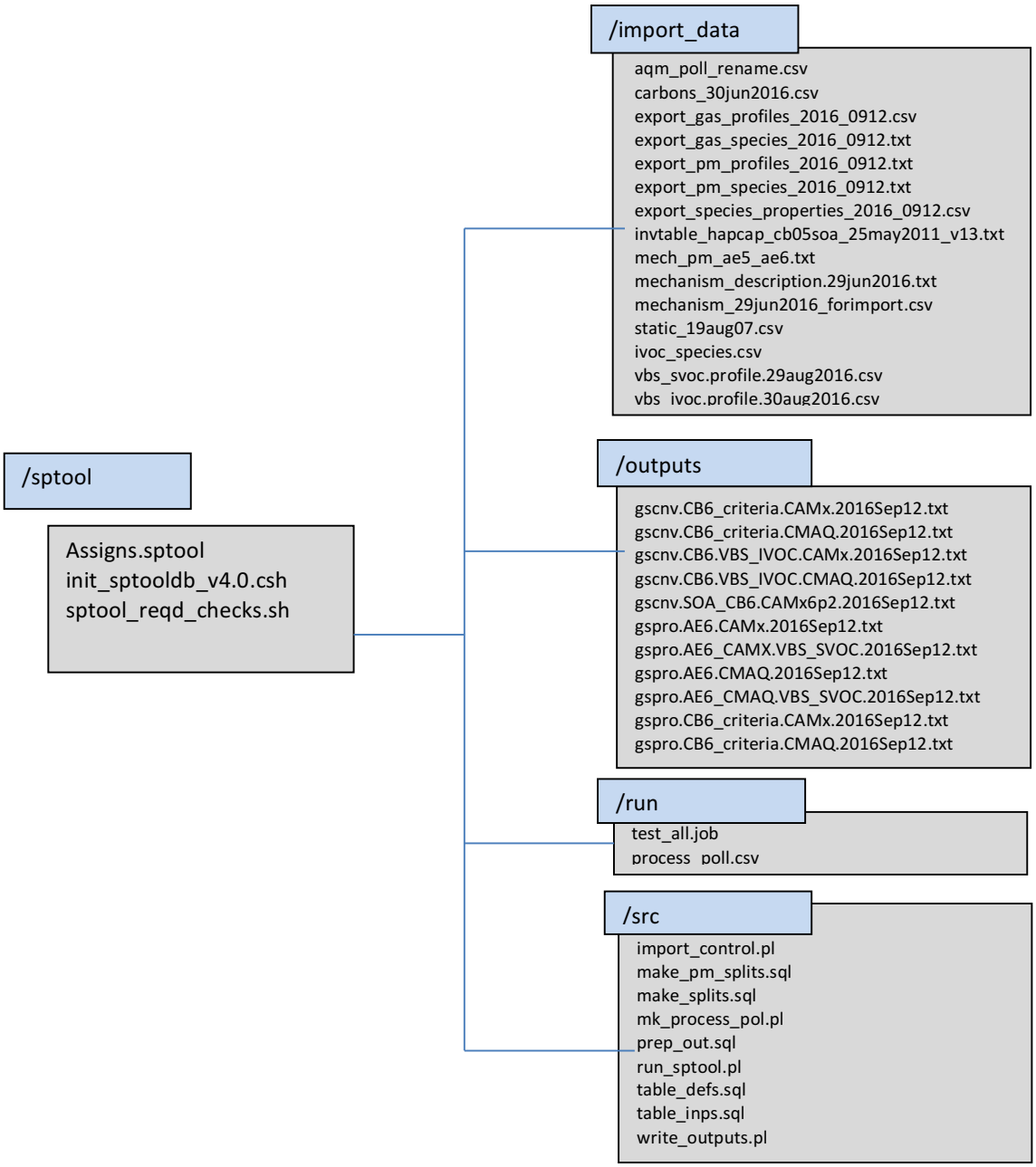


Exhibit 3-1. Speciation Tool Directory and File Names.

3.3 Check for required software

Before you begin the initialization, first verify that PostgreSQL and Perl are installed and accessible. Whoever is installing the Speciation Tool requires PostgreSQL permission to create a database. Execute the script *sptool_reqd_checks.sh* to check that the required software can be found and to verify user PostgreSQL authorizations.

```
> ./sptool_reqd_checks.sh
```

Following is an example of a successful check for the required software:

```
===== Speciation Tool Requirements Check =====

Checking the status of software requirements...

Status of required software:
[x] = Installed
[ ] = Not installed
[?] = Unable to determine, see notes

------PERL------
[x] Perl
[x]   -DBI
[x]   -DBD-Pg
[x]   -Text-CSV

---POSTGRESQL---
[x] PostgreSQL
[x]   -PL/pgSQL

Refer to the Speciation Tool User Guide Appendix A for installation procedures of the required software.
```

3.4 Initialize the Speciation Tool Database

Prior to making any Speciation Tool runs the Speciation Tool must be initialized. First, set the required environment variables and then start the initialization.

3.4.1 Update and source the *Assigns.sptool* file

The *Assigns.sptool* file provided in the top level Speciation Tool home directory sets environment variables that are required for initialization. These include the Speciation Tool home directory, database name, and input file names of the default speciation data. The only environment variable that must be updated is SPTOOL_HOME. This is installation dependent and must be set based on your system. Change the path name to correspond to the directory where the Speciation Tool top directory resides on your system. For example, if you install the Speciation Tool under the directory /disk4/models/emis, you would set the SPTOOL_HOME environment variable like this:

```
setenv SPTOOL_HOME  /disk4/models/emis/sptool  # Speciation Tool top level directory
```

The other environment variable that you might want to change is the Speciation Tool database name. The file provided in the distribution package has this variable set to sptoolv4_0:

```
setenv SPTOOL_DB        sptoolv4_0              # Speciation Tool Database name
```

You may change "sptoolv4_0" to any valid PostgreSQL database name; just be sure it doesn't currently exist. The command line 'psql –l' (dash lower case L) will display a list of existing PostgreSQL databases. Restrict the database name characters to a – z, 0 – 9, and the underscore "_" with no imbedded blank characters.

When the *Assigns.sptool* file has been updated then 'source' the file to set the required environment variables.

```
> source Assigns.sptool
```

3.4.2 Create the Speciation Tool database

The initialization script, *init_sptooldb_v4.0.csh*, is a C-shell script that checks for required environment variables, executes a set of PostgreSQL commands to create the Speciation Tool database, sets database permissions, creates the *shared* schema and table definitions for the tool data, imports Speciation Tool SQL functions and data to the *shared* schema. The functions imported by the script perform the computations needed for generating the speciation profiles and pollutant-to-pollutant factors that are output by the program.

```
>./init_sptooldb_v4.0.csh
```

Messages are printed to the screen to reflect installation progress. The first part of a successful initialization will look similar to:

```
>./init_sptooldb_v4.0.csh

SPTOOL_SRC_HOME = /disk4/models/emis/sptool/src
New database: SPTOOL_DB = sptoolv4_0
SPTOOL_USER = yourusername
POSTGRES_BIN = /usr/local/pgsql/bin
CREATE DATABASE
Database sptoolv4_0 created
CREATE SCHEMA
Shared schema created
GRANT
Create permissions granted on sptoolv4_0
GRANT
All permissions granted on shared schema
Defining custom functions and initializing tables.  ...working



 Speciation Tool functions and tables successfully defined in sptoolv4_0.
```

If you forget to set the environment variables you will get error messages as displayed below. Review the previous section on the *Assigns.sptool*, source the Assisgns file, and then rerun the initialization script.

```
SCRIPT ERROR: Required environment variable SPTOOL_SRC_HOME not set
        in script init_sptooldb_v4.0.csh
SCRIPT ERROR: Required environment variable SPTOOL_DB not set
        in script init_sptooldb_v4.0.csh
ABORT: init_sptooldb_v4.0.csh script aborted with errors.
```

If you attempt to initialize the Speciation Tool with a database name that already exists you will get the following message:

```
createdb: database creation failed: ERROR:  database "sptoolv4_0" already exists
ERROR: failed to create a new database sptoolv4_0. This usually means the database already exists.
        To replace the existing database type 'dropdb sptoolv4_0' from the command line.
```

Delete the existing database if you want it replaced. Otherwise change the SPTOOL_DB name in the Assigns.sptool file and provide a different database name. The command to delete the existing PostgreSQL database is:

```
> dropdb $SPTOOL_DB
```

Once you either drop the existing database or change the assigned name you can start the initialization again.

3.4.3 Load the Speciation Tool *shared* schema data

The final step in initializing the Speciation Tool is to load the data that is provided in the distribution package. This information includes species properties, chemical mechanism definitions, speciation profile definitions from SPECIATE 4.5, and some additional general information that is shared by all Speciation Tool runs. The data are imported to the Speciation Tool database during initialization and stored in tables in the Speciation Tool PostgreSQL database *shared* schema.

A database contains one or more named schemas, which in turn contain tables and other objects. The same table name can be used in different schemas without conflict; for example, in Exhibit 2.1 both cb05_criteria and saprc_toxics schemas contain the same table names. Unlike PostgreSQL databases, schemas are not rigidly separated; a user can access tables in any of the schemas within the same database. The Speciation Tool *shared* schema is accessed by all Speciation Tool runs; the tables are shared.

The input data files reside in the /import_data subdirectory of the Speciation Tool home directory. The file names are assigned to environment variables in the *Assigns.sptool* file and do not need to be changed.

Messages are displayed during the initialization process to indicate progress while importing the shared data. Below is a partial sample of a successful load. The time it takes to import the data will vary depending on your system, a few minutes is typical.

```
Importing mechanisms  /disk4/models/emis/sptool/src/../import_data/mechanism_mar2013_forimport.txt

Using transactions - import of data will abort on any error.
Reading data from /disk4/models/emis/sptool/src/../import_data/mechanism_mar2013_forimport.txt...
  1000 lines processed
  2000 lines processed
...
  18000 lines processed
...finished, imported 18981 lines.

...

Importing species properties /disk4/models/emis/sptool/src/../import_data/export_species_properties_2013_0311.csv

Using transactions - import of data will abort on any error.
Reading data from /disk43/sptool/wa1_05.2012/src/../import_data/export_species_properties_2013_0311.csv...
  1000 lines processed
  2000 lines processed
...finished, imported 2274 lines.

Speciation Tool shared data successfully imported

Completed:  Wed Sep 20 11:50:30 PDT 2016
```

The Speciation Tool uses the *shared* schema functions and tables in every run. Appendix B provides the table definitions that are stored in the *shared* schema.

If an error occurs while importing the data the program will terminate with a message indicating which file and record caused the error. A database rollback will be initiated and none of the data for the file with the error will be imported. The import stops at the first error.

3.4.4 The Import Program

The initialization script executes the Perl program *import_rawdata.pl* for each file imported to the *shared* schema. Each database table in the *shared* schema is associated with a keyword listed in Table 1 which identifies the table to populate. To import additional data to the *shared* schema tables you can execute the Perl program from the command line. This will essentially append data to an existing table.

```
> perl $SPTOOL_SRC_HOME/import_rawdata.pl  $SPTOOL_DB  table_type  input_file
```

The parameters include the database name, a keyword from Table 1, and the path/file name of the inputs records. The input data must conform to the table definitions in Appendix B. Any error will abort the import with a database rollback; no records will be appended to the table.

Table 1. Keyword list showing Speciation Tool *shared* data types.

Keyword	Description
mechanism	mechanism definition
mechanismPM	$PM_{2.5}$ mechanism definition
mechanism_description	description and data source for each chemical mechanism
invtable	SMOKE Inventory Table
gas_profiles	gas profile description and historical information
gas_profile_weights	gas weight profiles
pm_profiles	PM profile description and historical information
pm_profile_weights	PM weight profiles
rename_species	rename mechanism AQM lumped species names
species	species data: ids, names, MW, etc
carbons	number of carbons for AQM lumped species name
static	static profiles, profile weights do not change
camx_fcrs	list of profiles where FPRM is renamed to FCRS
vbs_svoc_factors	SVOC factors by profile for VBS modeling
vbs_ivoc_factors	IVOC factors by profile for VBS modeling
ivoc_species	molecular weights for IVOC compounds

After a successful Speciation Tool initialization, the PosgreSQL *sptoolv4_0* database will be created with the *shared* schema that holds the tool functions and default data.

4.0 RUNNING THE SPECIATION TOOL

A Speciation Tool run will generate the speciation factors required to convert emission inventory compounds (e.g. VOC or $PM_{2.5}$) to lumped modeling compounds (e.g. OLE or ALD2) for air quality modeling. This chapter discusses the mechanics of running the Speciation Tool, which include how to run the tool and the parameters and options available.

The command to run the Speciation Tool is:

```
perl $SPTOOL_SRC_HOME/run_sptool.pl <database> <run_name> <run_control_file>
```

The command line parameters include the database name, user specified run name, and a control file. The *run_sptool.pl* program creates the run schema, reads and imports the specified control file, imports run-specific data files, executes the PostgreSQL functions to compute the split factors and conversion factors, and writes the output files.

Prior to running the Speciation Tool:

- Source the Assigns file
- Create a Run Control file
- Develop the input files that are required for the run

4.1 The Run Script

The Perl program *run_sptool.pl* creates the output speciation profile files GSPRO and GSCNV. The program requires the source code directory and database name. Source the *Assigns.sptool* file to set the required environment variables SPTOOL_HOME and SPTOOL_DB. This file is discussed in the previous chapter on initializing the Speciation Tool.

If you receive an error "file not found" when running the script, it is probably because you have not set the Speciation Tool home directory or that the path is set to an invalid path name.

4.2 Run Name

The run name is an identifier to uniquely label the Speciation Tool run. It is used to create a schema of that name in the Speciation Tool database. To create a new schema, specify a run name that has not previously been used. If you specify an existing run name then the existing schema is dropped and replaced by the new run.

The run name must meet the following conditions:

- Begin with an alphabetic character
- Must **not** include spaces in the name
- Must **not** be the *'shared* ' schema
- Should be different from all existing run identifiers in the Speciation Tool, unless an existing run is meant to be replaced

- Must **not** be 'public' or begin with 'pg_' which are reserved for system schemas
- Must be less than 64 characters in length

The command to list existing schema (runs) in the database is:

```
psql   <database_name>   -c   'select * from pg_namespace'
```

where <database_name> is the Speciation Tool database name. The first column of the resulting list, labeled nspname, will include run names as well as system schema names. The last column, labeled nspacl, lists the owner of each schema.

4.3 Run Control File

The run control file indicates the run parameters and the run-specific data files required for a Speciation Tool run. The format of the run control file is

<keyword>, <option>

Only lines that begin with a keyword are recognized by the database. All other lines are skipped allowing imbedded comments within the control file. Table 2 summarizes the control file keywords and options. Details for each keyword are provided in following sections.

Table 2. Speciation Tool Control File Keywords.

Keyword	Description
Run Parameters	
MECH_BASIS	Mechanism identifier/name. Matches identifier in the shared schema mechanism table. Options provided with Speciation Tool include: • CBIV • CB05 • CB6 • SAPRC99 • SAPRC99B • SAPRC07 • SAPRC07T • SOA_CAMX45 • SOA_CAMX45_SP99 • SOA_CB6CAMX6P2 • AE5 • AE6
OUTPUT	Output options (default is VOC): • VOC • PM • STATIC
RUN_TYPE	Specifies how split factors are developed. Options include: • CRITERIA • INTEGRATE • NOINTEGRATE • HAPLIST

Keyword	Description
Run Parameters	
	• VBS
AQM	Air quality model. Determines some of the pollutant names for the output files. Options: • CAMX • CMAQ
TOLERANCE	The acceptable deviation for which the sum of weight percentages for a profile definition is within 100%. The default is 5%. Applies only to gas profiles.
Optional Input Files	
TOX_FILE	Toxic species path/file name.
PRIMARY_FILE	Additional toxic entries path/file name.
PROC_FILE	Mobile process modes path/file name.
PRO_FILE	User-defined input profiles path/file name.
Output Files	
SPLITS_OUT	Output speciation profiles (GSPRO) path/file name.
CNV_OUT	Output conversion factors (GSCNV) path/file name.

4.3.1 Run Parameters

MECH_BASIS Example: MECH_BASIS, CB05
This parameter indicates the chemical mechanism to use for mapping species to the AQM lumped modeling compounds. The specified mechanism must match a mechanism name in one of the mechanism tables in the *shared* schema which are imported when the Speciation Tool is initialized. The data provided with the Speciation Tool include VOC mechanism definitions for CBIV, CB05, CB6, SAPRC07, SAPRC07T, SAPRC99, SAPRC99B, SOA_CB6CAMX6P2, SOA_CAMX45, and SOA_CAMX45_SP99 and $PM_{2.5}$ mechanism definitions for AE5 and AE6.

OUTPUT Example: OUTPUT, VOC
The OUTPUT keyword indicates which output profiles will be generated. The output options are "VOC" gas species, "PM" particulates, and "STATIC". Only one option can be specified per run. STATIC represents the list of splits that do not change with profile weight definitions, such as the pollutants CO and NH3. It simply formats the imported static profiles to correspond to the output GSPRO file format.

The OUTPUT keyword is optional. If it is omitted from the control file the default is to generate VOC factors.

RUN_TYPE Example: RUN_TYPE, CRITERIA
The RUN_TYPE options are: CRITERIA, INTEGRATE, NOINTEGRATE, HAPLIST, and VBS.

> CRITERIA: All model species, including toxic species, are computed from criteria emissions.

INTEGRATE: The HAPs species are to be integrated from a separate emission inventory. Part of the criteria VOC mass is replaced with the HAP VOC mass. This involves subtracting toxic VOC emissions from the criteria VOC emissions to avoid double counting of VOC. Profiles are generated as NONHAPTOG.

NOINTEGRATE: The HAPs species from a separate inventory are not integrated. The criteria VOC mass retains the HAP VOC mass. The nointegrate approach occurs when the separate inventories do not have the necessary details to provide a one-to-one match. The **active** HAPs (specified as explicit in the INVTABLE) are removed from the VOC profiles but the profiles are not renormalized, mass is preserved, and profiles are generated as TOG.

HAPLIST: Generates records for the HAPs that define the SMOKE calculation of NONHAPTOG.

VBS: The Volatility Basis Set (VBS) option generates semi-volatile organic compounds (SVOC) when generating $PM_{2.5}$ profiles or intermediate-volatility organic compounds (IVOC) when generating VOC profiles.

The different run types support different simulation options in SMOKE. For emissions processing of only total VOCs the CRITERIA option is used. The INTEGRATE or NONINTEGRATE options are used if a separate toxics inventory is included in addition to a total VOC inventory in the SMOKE modeling. The INTEGRATE case will generate NONHAPVOC profiles in which the toxics mass is removed from the criteria VOC mass. The NOINTEGRATE case is selected when sources in the criteria inventory and the toxics inventory cannot be definitively matched. The NOINTEGRATE case assumes that the criteria VOC mass includes toxics mass. Refer to the SMOKE User's Manual (http://www.smoke-model.org) for more detailed information of how SMOKE handles integrating criteria VOC and toxics inventories.

Note: The Speciation Tool *shared* tables includes a default INVTABLE file. These data should be reviewed and potentially replaced with the INVTABLE that you are using for SMOKE modeling.

The only run types currently supported for $PM_{2.5}$ output is CRITERIA and VBS.

AQM Example: AQM, CAMX

The Air Quality Model (AQM) is used to determine the appropriate model species names in the output files. The Speciation Tool initialization data files support the AQM options CMAQ and CAMX. CMAQ stands for the Community Multiscale Air Quality Model, and the CAMX option stands for the Comprehensive Air Quality Model with extensions.

Different models sometimes use different names for the same species. For example, 'other' $PM_{2.5}$ emissions are mapped to the model species name "PMOTHR" in CMAQ and "FPRM" in CAMX. Tables tbl_static and tbl_rename_species in the shared schema include fields that indicate model-specific lumped species names. If another model uses different lumped species names then those cases need to be included in these tables. The shared schema table

tbl_rename_species allows you to export model-specific species names different from the ones specified in the mechanism table. For example, ethene in the SAPRC99 mechanism is stored as "ETHE" in the mechanism table and is mapped to the model species name "ETHENE" for CMAQ.

TOLERANCE Example: TOLERANCE, 3
Each profile is defined as the sum of its components and is quantified as the percent contribution of each component to total organic gases. Ideally the sum of the percent components for each profile should equal 100 percent, which means that all mass is accounted for and assigned to individual species. However, due to round-off or inaccurate profile definitions the sum of the profile components do not always add to 100%. The optional TOLERANCE keyword defines an acceptable deviation from 100%, with the default hard-coded in the Speciation Tool at 5%. Any profile definition where the sum of the percent is outside the acceptable tolerance will **not** be output in the run. In other words, all profiles that sum to less than 95% or greater than 105% are excluded from the output.

If the sum of the weight percentages for a particular profile is not 100% and nothing is done to correct the profile definition then the resulting speciation profile will drop or add mass if used in emissions modeling. The Speciation Tool renormalizes all gas profiles whose sum is within the tolerance thereby preserving VOC mass. Profiles outside of the tolerance are dropped at run time. These profiles are not included in the model outputs but they do continue to reside in the *shared* schema tables.

4.3.2 Input Files

File formats for all of the run specific input files are provided in Appendix C.

PRO_FILE Example: PRO_FILE, ctl/prfwts_02coalstudy.dat
The PRO_FILE keyword is used to specify a file of gas profiles. Specifying this option will override using the gas profiles defined in the *shared* schema. The profiles provided in this input file are the profiles for which the model will generate the splits and conversion factors. PRO_FILE is an optional keyword in the control file. The default is to use the profile definitions in the *shared* schema. At this time, only one set of profiles is used per run; either the *shared* data or the data provided using the PRO_FILE keyword. If speciation profiles are required from both sources then separate runs are required.

TOX_FILE Example: TOX_FILE, ctl/toxics_coalstudy.dat
The toxics file is required for run types INTEGRATE, NOINTEGRATE, and HAPLIST. The file lists the toxic compounds that are explicit in the chemical mechanism. The Speciation Tool uses the information in the Inventory Table, imported to the *shared* schema during initialization, to determine whether the toxics are to be treated as active or tracer compounds. An active compound is defined with 'Y' in the INVTABLE *explicit* field. Active species are included in the chemical mechanism with chemical feedback, while tracer species are included in the mechanism with no chemical feedback. Tracer toxics species mass is double counted.

For the INTEGRATE case (i.e., RUN_TYPE, INTEGRATE) the active and tracer toxic species are removed from the VOC profiles, whereas for the NOINTEGRATE case, only active toxic species are removed from the VOC profiles.

For the case where HAPLIST is the specified RUN_TYPE, the active HAPs produce a single one-to-one mapping from HAPs inventory pollutant to model compound. The tracer HAPs generate the same mapping as the active, but in addition, the HAPs inventory pollutant is mapped to the original VOC profile compounds to support the INTEGRATE case. The HAPLIST case also generates a 'nointegrate' HAP by appending the suffix "_NOI" to the model compound (for example, BENZENE_NOI).

The toxics file is only applicable to VOC output.

PRIMARY_FILE Example: PRIMARY_FILE, ctl/primary_toxics_coalstudy.dat
You can add or override toxic entries by providing a primary toxic list. This file is only used when the run type is HAPLIST. If it is specified for any other run type the data are ignored.

The overwrite flag carried in this table determines whether a toxic species should be added ("N") or replaced ("Y") in the GSPRO file. This capability allows the Speciation Tool to support the one-to-many toxics species mapping and primary toxic profiles. The file format and example are as follows:

```
<Inv poll> <AQM name>    <splitfac> <overwrite flag>
FORMALD,   FORM_PRIMARY,   1.0,     N
ACETALD,   ALD2_PRIMARY,   1.0,     N
XYLS,      MXYL,           0.52,    Y
XYLS,      OXYL,           0.16,    Y
XYLS,      PXYL,           0.16,    Y
```

The overwrite flag in the last column determines whether a toxic species should be added ("N") or replaced ("Y") in the GSPRO file. XYLS (species id = 507) in the input toxic table has been assigned to DONT_USE (any place holder would suffice). With the overwrite flag turned on, the Speciation Tool will remove the "XYLS DONT_USE" entry and add the three XYLS entries shown above. The FORM_PRIMARY and ALD2_PRIMARY will be added to the GSPRO.

PROC_FILE Example: PROC_FILE, process_mode.dat
The PROC_FILE keyword specifies an optional input file which provides mobile source emission modes for profiles that represent mobile processing. This feature is provided to support SMOKE requirements of mobile source emission modes. An example record in this file is "4674, EXH" where profile code 4674 applies to exhaust emissions. When the process file is provided then additional records are generated in the GSCNV output file. For example, profile 4674 would include a VOC to TOG record as well as an EXH_VOC to EXH_TOG record; with the same conversion factors.

4.3.3 Output Files

SPLITS_OUT Example: SPLITS_OUT, outputs/gspro_02coalstudy.dat
The SPLITS_OUT keyword is used to optionally specify a path and file name for the model splits results written in SMOKE GSPRO format. Paths can be relative paths from the Speciation Tool main directory (as shown) or absolute paths. This is an optional keyword. If omitted the output file name is derived from the run control parameter specifications and the run date and is written to the relative path /outputs. An example of a default output filename is outputs/gspro_CB05_NOINTEGRATE_CAMX_26Jun2011.

CNV _OUT Example: CNV_OUT, outputs/gscnv_02coalstudy.dat
The CNV_OUT keyword is used to optionally specify a path and file name for the model TOG/VOC conversion factors written in SMOKE GSCNV format. Paths can be relative paths from the Speciation Tool main directory (as shown) or absolute paths. This is an optional keyword. If omitted the output file name is derived from the run control parameter specifications and the run date and is written to the relative path /outputs. An example of a default output filename is outputs/gscnv_CB05_NOINTEGRATE_CAMX_26Jun2011.

4.3.3.1 Header Records: Metadata

The Speciation Tool output files, GSPRO and GSCNV, contain header records which are referred to as 'metadata'. Each of the output files has the same common metadata keywords. The purpose of the metadata records is to provide a summary of the data and parameters that were used to generate the outputs. Table 3 provides the list of metadata keywords for an example run.

Table 3 Metadata keywords and example.

Metadata Keyword	Example
#SPTOOL_AQM	CMAQ
#SPTOOL_CARBONS	carbons_cb6_cb05_cbiv_saprc99.csv
#SPTOOL_GAS_PROFILES	Qry_gas_specie_export.txt
#SPTOOL_INVTABLE	invtable_caphap_27jun2007_v7.txt
#SPTOOL_MECH	CB05
#SPTOOL_PM_PROFILES	Not Applicable
#SPTOOL_PROCESS	process_poll.csv
#SPTOOL_STATIC	Not Applicable
#SPTOOL_VOC_TYPE	INTEGRATE
#SPTOOL_CAMX_FCRS	Not Applicable
#SPTOOL_VBS_SVOC_FACTORS	Not Applicable
#SPTOOL_VBS_IVOC_FACTORS	Not Applicable

If the keyword is not applicable for a particular run then the corresponding value is set to "Not Applicable". For example, if the output type is specified as PM then the metadata record #SPTOOL_GAS_PROFILES is set to "Not Applicable". These headers can be used as a guide for merging different GSPRO tables. Before combining outputs for toxics TOG profiles with NONHAPTOG profiles one should confirm that the same chemical mechanism was specified for each run and that the same input files for the VOC calculations were used for each run.

4.4 Run the Speciation Tool

To run the Speciation Tool, enter the following command:

```
perl $SPTOOL_SRC_HOME/run_sptool.pl $SPTOOL_DB <run_name> <run_control_file>
```

Where:

$SPTOOL_DB is the Speciation Tool database name
<run_name> is the user assigned run name
<run_control_file> is the name and location of the control file which defines the run parameters and input and output file names.

4.4.1 Run-time Messages

The Speciation Tool writes a number of messages to standard output that indicate the program progress. The messages indicate key steps as they are completed either from the Perl scripts or the PostreSQL functions. The difference between the message types is easily detected as all of the PostgreSQL messages begin with the word "NOTICE". Exhibit 4-1 provides an example of a typical list of run-time messages. This example is for the run identified as "cb05_integrate". If a run name is specified for a case that has been previously run, then additional messages are written at the start of the program that indicate existing tables are being dropped. For example, "NOTICE: drop cascades to table cb05_integrate.tmp_metadataset".

```
Created cb05_integrate schema
Granted permissions on cb05_integrate schema
Set path successfully to cb05_integrate schema
Input tables created in cb05_integrate schema
Completed importing User Profile Weights file user_prof_wts_2540.txt
Imported run control file run_ctl_cb05_integrate.txt in cb05_integrate schema
NOTICE:  Type of Output is  VOC
NOTICE:  AQM is  CAMX
NOTICE:  Type of run is  INTEGRATE
NOTICE:  Mechanism basis is  CB05
NOTICE:  Profile Tolerance is  5
NOTICE:  ...establishing profile weights
NOTICE:  ...renormalizing profile weights
NOTICE:  ...establishing mechanism
NOTICE:  ...calculating moles per gram emissions
NOTICE:  ...calculating mole percent
NOTICE:  ...calculating moles per mole emissions
NOTICE:  ...summing on AQM pollutant
NOTICE:  ...calculating mole weight percent
NOTICE:  ...calculating average molecular weight by specie
NOTICE:  ...calculating average molecular weight by AQM
Completed splits calculations
Completed output preparations
Completed writing the output files for run cb05_integrate
```

Exhibit 4-1. Example of run-time messages.

There are a number of different warning messages that are displayed during processing. The most frequent message occurs when a species exists in the *shared* schema species table that has not been defined in the specified chemical mechanism. Below is a small example of these messages which provide the Species ID number and name. There are many species that are currently undefined in the chemical mechanisms. This is only a concern if a profile references one of them.

```
NOTICE:  WARNING review vvvvvvvvvvvvvvvvvvvvvvvvvvvvvvvvvvvvvvvvvvvvvvvvvvvvvvvvvvvvvvvvvvvvvvv
NOTICE:  WARNING: CB6 mechanism undefined for the following species.
NOTICE:         The following will be set to UNK if referenced.
NOTICE:  WARNING:        SPECIES ID  2673 2,6-dimethylheptane, propylcyclopentane
NOTICE:  WARNING:        SPECIES ID  2674 Trans-3-hexene; 3-methylcyclopentene
NOTICE:  WARNING:        SPECIES ID  2675 2-methyl-2-hexene; cis-3-heptene
NOTICE:  WARNING:        SPECIES ID  2676 3-methyl-trans-3-hexene; Trans-2-heptene
```

Profiles are dropped during processing when the weight percent sum is outside the specified tolerance. The dropped profiles are reported to standard output. Below is a small example of these warnings.

```
NOTICE:  ...establishing profile weights
NOTICE:  WARNING review vvvvvvvvvvvvvvvvvvvvvvvvvvvvvvvvvvvvvvvvvvvvvvvvvvvvvvvvvvvvvvvvvvvvvvv
NOTICE:  WARNING The following profiles were dropped.
NOTICE:  WARNING Total weight percent is outside the tolerance of 5 percent.
NOTICE:  WARNING:   PROFILE ID  4742 82.87586700 percent Diesel Exhaust - Bus at -10 oC, 2-stroke
NOTICE:  WARNING:   PROFILE ID  4743 83.00138200 percent Diesel Exhaust - Bus at 20 oC, 2-stroke
NOTICE:  WARNING:   PROFILE ID  4744 84.50961700 percent Diesel Exhaust - Bus at -10 oC, 2-stroke, oxidatio
```

Many of these listed profiles have a profile definition with a percent sum of 100%. The problem is not with the profile definition but the incomplete species data. Any species with an undefined molecular weight is dropped from the profile since the molecular weight is required to compute the splits factors. This dropped percent due to missing molecular weights sometimes takes the total profile percent sum outside the accepted tolerance. This type of problem can be resolved by updating the species properties molecular weights.

The complete list of undefined species in a chemical mechanism can be quite long. An additional list of undefined species that are referenced by a profile, whose weight percent will be assigned to UNK is also provided. This is a small subset of the complete list of species that are not defined in the chemical mechanism.

```
NOTICE:
NOTICE:  WARNING review vvvvvvvvvvvvvvvvvvvvvvvvvvvvvvvvvvvvvvvvvvvvvvvvvvvvvvvvvvvvvvvvvvvvvvvvvvvvvvv
NOTICE:  WARNING: CB6 mechanism undefined for the following species.
NOTICE:       The following species are referenced by profiles and will be set to UNK.
NOTICE:  WARNING:       SPECIES ID  1014 2-pentylfuran
NOTICE:  WARNING:       SPECIES ID  2715 Cyclopropane
NOTICE:  WARNING:       SPECIES ID  2716 1-Chloro-3-methylbenzene
```

4.4.2 What happens when the script is running?

The *run_sptool.pl* program creates the run schema, reads and imports the run control file, imports the run-specific data files, executes the PostgreSQL functions that compute split factors and conversion factors, and writes the output files. After the script has been run, the run-specific schema retains the run parameters, input data, intermediate calculations, and the final results. Appendix C lists the run-based schema table formats for the input data and a list of the database tables created during a run.

The Speciation Tool is driven by the Perl program *run_sptool.pl*. Table 4 provides a summary of the program steps.

Table 4. Program and module calls from the Speciation Tool program, run_sptool.pl.

Command line	Language	Description
SELECT inputs_createtables	SQL	Executes PostgreSQL commands in table_inps.sql: • Creates tables in the run-id schema.
import_control.pl	Perl	Imports the run control data and optional user specified input data.
SELECT MakeSplits	SQL	If VOC processing: Executes PostgreSQL commands in make_splits.sql: • Creates tables in the run_id schema. • Performs data validity checks. • Performs numerous calculations to generate the gas split factors.
SELECT MakePMSplits	SQL	If $PM_{2.5}$ processing: Executes PostgreSQL commands in make_pm_splits.sql: • Creates tables in the run_id schema. • Performs data validity checks. • Performs calculations to generate the $PM_{2.5}$ split factors
SELECT PrepOut	SQL	Executes PostgreSQL commands in prep_out.sql: • Creates tables in the run_id schema. • Generates the output splits and conversion factors data.
write_outputs.pl	Perl	Extracts from the run_id schema the split factors and conversion factors data and writes the output GSPRO and GSCNV files.

In addition to the above commands numerous data and processing checks are performed in the run script.

5.0 APPLICATIONS AND METHODOLOGY

The Speciation Tool generates emission modeling speciation profiles formatted for SMOKE. The data files provided with the Tool include gas profiles, PM profiles, and a comprehensive species list extracted from EPA's SPECIATE 4.5 database. In addition, chemical mechanisms used in Air Quality Models CMAQ and CAMx are also provided. These data are the building blocks to generating speciation profiles.

The Speciation Tool can produce either gas profiles or $PM_{2.5}$ speciation profiles.

5.1 Gas profile processing

The Speciation Tool is designed to support the availability of both CAPS and HAPS, to either integrate the HAPs in the chemical mechanism or not, and to include both active and tracer species in modeling. It is designed to generate the GSPRO and GSCNV speciation input files for the SMOKE model. Refer to the SMOKE User's Manual for detailed information of how SMOKE handles integrating the criteria VOC and toxics inventories.

The Speciation Tool *shared* schema includes the table *tbl_invtable* which carries the imported default INVTABLE data. These data should be reviewed to verify that they correspond to the SMOKE INVTABLE that will be used in your SMOKE modeling.

5.1.1 Run Type Options

The different Speciation Tool run options for gas profile processing are: CRITERIA, INTEGRATE, NOINTEGRATE, HAPLIST, and VBS. CRITERIA is specified if no additional HAPS inventory is included in the modeling. The INTEGRATE and NOINTEGRATE options indicate how a separate HAPS inventory will be handled in the SMOKE model by either subtracting the HAPS portion from the criteria VOC or not. The HAPLIST option generates the HAPS records used in SMOKE for computing NONHAPVOC. VBS is a CRITERIA run where a portion of the non-methane mass is assigned to IVOC compounds.

5.1.1.1 CRITERIA

A run type of CRITERIA means that all VOC model species, including toxic VOC species, are computed from criteria VOC emissions. This option is specified when there is not a separate toxics emissions inventory included in modeling.

5.1.1.2 INTEGRATE

A run type of INTEGRATE means that the specified HAPs species are integrated from a separate emission inventory. Part of the criteria VOC mass will be replaced with the HAP VOC mass from the HAP emission inventory. SMOKE computes the NONHAPVOC mass from the criteria VOC mass by subtracting the HAP VOC mass.

The Speciation Tool creates the HAPs list using the Inventory Table data which is imported during initialization. The HAPs list is composed of species/compounds in the Inventory Table where the field Keep = Y **AND** the field VOCTOG = (V **OR** T). The HAPs are removed from the

VOC profiles and the profiles are renormalized and generated as NONHAPVOC profiles. The GSCNV output file will contain NONHAPVOC to NONHAPTOG factors.

The GSPRO header records list all of the toxic species that are subtracted from TOG to estimate NONHAPTOG. If the Inventory Table includes process mode information for on-road mobile modeling then some pollutant names will also be appended to the process mode. For example,

```
#NHAP NONHAPTOG BENZENE
#NHAP NONHAPTOG EVP__BENZENE
```

SMOKE compares the INVTABLE settings to the header records in the GSPRO file ensuring that the lists are consistent.

5.1.1.3 NOINTEGRATE

In the NOINTEGRATE case both the criteria VOC inventory and the separate toxics inventory are included in emissions processing. However, due to an inability to map one inventory to another, toxics are included from both sources. The criteria VOC includes the HAP VOC mass. In generating the speciation profiles, the specified **active** HAPs are removed from the VOC profiles but the profiles are not renormalized, mass is preserved, and profiles are generated as VOC.

5.1.1.4 HAPLIST

This option generates records for the HAPs that define the NONHAPVOC for both the INTEGRATE and NOINTEGRATE cases. All HAPS are written to profile number '0000' which is often used as the default profile ID in SMOKE processing.

5.1.1.5 VBS

The VBS (Volatility Basis Set) option produces intermediate-volatility organic compounds (IVOC) and adjusted non-methane organic gas (NMOG) components for CRITERIA gas processing. IVOC represents VOC with volatility ranging from 10^3 to 10^6 µg/m^3. The Speciation Tool default input data includes a table of profile codes and the fraction of NMOG that is assigned to IVOC for each profile. When IVOC is added the VOC model species is reduced so that total NMOG mass is conserved. Currently (2016) about 20% of gas profiles output IVOC compounds.

5.1.2 Chemical Mechanisms

During initialization the Speciation Tool imports default data (profiles, species list, chemical mechanism, etc) into the *shared* schema. However, the Speciation Tool is not tailored to a specific chemical mechanism such as CB05. If the chemical mechanism you require is not available in the Speciation Tool database you can import a new mechanism definition, assuming you can supply the new chemical mechanism assignments. Refer to the Chapter FAQ for these details.

The Speciation Tool also has the capability to generate speciation profiles for secondary organic aerosols (SOA) to support air quality models such as CAMx that have an explicit SOA scheme.

This is accomplished through the use of one of the chemical mechanisms included in the initialization data. For example, SOA_CB6CAMX6P2, defines the secondary components TOLA, XYLA, BNZA, ISP, and TRP for the CB6 mechanism in CAMx versions 6.2 and later.

When using the SAPRC99 mechanism keep in mind that the carbon content of VOC or TOG emissions is not conserved through the SAPRC99 speciation step, that the output mass fractions in the GSPRO file are sensitive to the number of carbons assumed for each species, and that carbon numbers are not well-defined for SAPRC99 lumped species. This uncertainty does not influence the output modeling emissions in molar units. Output emissions reported in mass units (such as speciated SMOKE reports) do inherit this uncertainty and, therefore, should be considered as qualitative rather than quantitative information.

5.2 $PM_{2.5}$ profile processing

The Speciation Tool supports speciation profile entries for $PM_{2.5}$. The CRITERIA and VBS run options are supported for PM processing. The chemical mechanism definitions imported during initialization include the CMAQ aerosol mechanisms AE5 and AE6. Appendix D provides these mechanism definitions. The Speciation Tool processes profiles with a lower bound size of 0 and an upper bound size of 2.5, all profiles outside these conditions are ignored.

The $PM_{2.5}$ chemical mechanism definitions include a list of species that define the mechanism, a flag ('qualify') to define the species that determine which profiles to process, and the AQM pollutant name to be assigned any unspecified PM mass (e.g. PMFINE).

A profile is processed if it contains one or more species that are flagged 'qualify'. For each profile that matches the selection criteria, only the species that are specifically defined in the chemical mechanism definition will be included in the outputs. Each $PM_{2.5}$ chemical mechanism definition is required to have one record specifying the AQM pollutant to compute. The unspecified mass component of each profile is defined as 1.0 minus the sum of the mass fractions of the mechanism compounds and is assigned to the 'compute' AQM pollutant. In the AE5 chemical mechanism the unspecified mass is assigned to PMFINE and in AE6 it is assigned to PMOTHR.

5.2.1 Special Handling for CAMx Particulate Modeling

As stated above the AE5 and AE6 aerosol mechanisms were developed specifically for CMAQ. In order to support CAMx PM speciation scheme (scheme CAMx CF), the Speciation Tool calculates the PM model species required by CAMx from the AE6 definition. Table 5 shows the relationship between CAMx CF scheme model species and the AE6 compounds.

Table 5. $PM_{2.5}$ components from CMAQ to CAMx.

CMAQ AE6 compounds	CAMx CF
PAL	sum >> FPRM
PCA	
PFE	
PK	
PMG	
PMN	
PMOTHR	
PSI	
PTI	
PNCOM	sum >> POA
POC	
PEC	PEC
PNA	NA
PH2O	PH2O
PNH4	PNH4
PNO3	PNO3
PSO4	PSO4
PCL	PCL
POC	POC*

* Note that POC is accounted under the CAMx POA compound. Although CAMx ignores POC, it is still included as a separate compound to assist with model performance evaluation.

5.2.2 Volatility Basis Set (VBS)

The VBS schemes include three distinct sets of SVOC model species to represent emissions from cooking (charbroiling), biomass-burning and other anthropogenic sources. Each SVOC model species set has five model species each with a different saturation pressure ranging from zero (non-volatile) to 1000 µg/m3 (most volatile).

The Speciation Tool needs new input data to support generating SVOC model species. Each profile code must be assigned to one of the three emission categories (cooking induced, biomass-burning, other anthropogenic), and SVOC species fractions for each saturation concentration bin. A Speciation Tool input table has been defined to map each PM profile code to fractions by saturation bin. SVOC species will replace the traditional POA for CAMx or POC and PNCOM for CMAQ. The five bin fractions must sum to one in order to conserve mass. The Speciation Tool checks the sum during processing and will abort if a record is found where the sum of the fractional components is not equal to 1.0.

6.0 FAQ

6.1 How do I add a single speciation profile?

The easiest method of processing one or more new profiles is to use the run control keyword pro_file. The profile definition is imported to a run schema table. If this table is populated then only profiles in the run schema are processed.

6.2 Can I have more than one copy of the Speciation Tool database?

Yes. If you want to rerun the Speciation Tool initialization and keep an already existing instance of the Speciation Tool database then all you need to do is make a copy of the *Assigns.sptool* file and change the database name variable SPTOOL_DB. 'Source' the new Assisgns file and run the initialization program. A new database is created and the specified data files imported.

This is the approach to take if you want to modify any of the shared data. In particular, you may have different versions of the INVTABLE that you want to support. Each version can be represented in a different database.

6.3 How do I define a new chemical mechanism?

To introduce a new chemical mechanism to the Speciation Tool first define the assignments to the mechanism table with a unique mechanism name (different from existing mechanisms) and import the data to the shared schema mechanism table (tbl_mechanism for VOC processing, tbl_pm_mechanism for $PM_{2.5}$ processing).

Next, the *shared* schema carbon table (tbl_carbons) may need to be updated to include any new model species names. The last step is to update the mechanism description table (tbl_mechanism_description) also in the *shared* schema.

For examples of the tables used to define new chemical mechanisms look under the import_data directory in the Speciation Tool distribution package for the following files:

tbl_mechanism: mechanism_14may2013_forimport.txt
tbl_carbons: carbons_14may2013.csv
tbl_mechanism_description: mechanism_description.14may2013.txt

Refer to Appendix B for the file formats.

The new mechanism data can be imported with the *import_rawdata.pl* Perl program.

```
perl  $SPTOOL_SRC_HOME/import_rawdata.pl $SPTOOL_DB  table_type  input_file
```

table_type - is the keyword from Table 1 (in this example it will be either mechanism, carbons, or mechanism_description)
input_file - contains the specified new records

Alternatively, rather than appending records to three separate shared schema tables (tbl_mechanism, tbl_carbons, tbl_mechanism_description) a new version of the Speciation Tool can be generated (refer to the question above). The new mechanism definition data could be imported as part of the initialization process. These data could be appended to existing files or not – depending on your processing preferences.

6.3.1 Example of how to introduce a new mechanism, "SAPRC99 with explicit benzene"

Update the mechanism table:

Extract the SAPRC99 entries from the import file

```
grep ^SAPRC99 mechanism_mar2013_forimport.txt > mechanism_saprc99_wexpl_benz.txt
```

Edit the new file:

Change SAPRC99 to SAPRC99_BENZ (on all records)
Delete existing benzene (specie_id = 302) assignments of "ARO1" and "NROG"
Add explicit benzene entry "SAPRC99_BENZ, 302, BENZ, 1."

Import the new mechanism file to the shared mechanism table

```
perl import_rawdata.pl database_name mechanism mechanism_saprc99_wexpl_benz.txt
```

Update the carbon table:

Create a file with the record "SAPRC99_BENZ,BENZ,6"
Import the file to the shared carbon table

```
perl import_rawdata.pl database_name carbons <new_carbon_file.txt>
```

Update the mechanism description table:

Create a file with the record "SAPRC99_BENZ, SAPRC99 with explicit benzene, Y, <description>,,"
Import the file to the shared mechanism description table

```
perl import_rawdata.pl database_name mechanism_description <new_file.txt>
```

The mechanism description table carries the field "NONSOA Flag" which defines whether the mechanism treats SOA explicitly. The CBIV, CB05 and SAPRC99 all have NONSOA Flag set to "Y". Only the SOA_CAMX45 mechanism has the flag set to "N".

6.4 What if I have a different INVTABLE?

The SMOKE INVTABLE data is imported as part of the Speciation Tool initialization. Currently there is not an optional input of this data for a single run. If you only need your version of the INVTABLE then replace the INVTABLE filename that is referenced in the Assigns.sptool before you initialize the database.

If you need multiple versions for your processing applications then you will need multiple versions of the Speciation Tool database; each importing a different INVTABLE during initialization. (Refer to 6.2 above).

6.5 How do I add a new species to the database?

To add a single record to the data base from the command line use an INSERT statement. The *shared* schema *tbl_species* carries almost twenty fields (exported from the SPECIATE database). The Speciation Tool references only a few of these fields. The required fields are specie_id, specie_name, volatile_mw, and non_voctog. Here is an example to add a single record to the table with only the required fields:

```
psql –d $SPTOOL_DB –c "INSERT INTO shared.tbl_species
                          (specie_id,specie_name,volatile_mw,non_voctog)
                   VALUES ('EG1', 'Example Name', 70.273,FALSE)"
```

The specie_id must be unique in the table; you will get an error if you attempt to add an already existing *specie_id*. The *non_voctog* field is type Boolean and should be set true if a TOG species is not regarded as a VOC.

APPENDIX A

PostgreSQL and Perl Installation Procedures

Linux Installation

This section provides the details for installing PostgreSQL and the required Perl modules (DBI, DBD-Pg, and Text-CVS) via the Linux command line. Before continuing it is recommended that you discuss these software requirements with your system administrator as you may need to be logged in as `root`.

Status of Requirements

Begin by checking what is or is not installed on your system. Execute the script *sptool_reqd_checks.sh* which is provided in the Speciation Tool package. The script checks for the required software and user PostgreSQL authorizations.

```
> ./sptool_reqd_checks.sh
```

Following is an example of a successful check for the required software:

```
===== Speciation Tool Requirements Check =====

Checking the status of software requirements...

Status of required software:
[x] = Installed
[ ] = Not installed
[?] = Unable to determine, see notes

------PERL------
[x] Perl
[x]   -DBI
[x]   -DBD-Pg
[x]   -Text-CSV

---POSTGRESQL---
[x] PostgreSQL
[x]   -PL/pgSQL

Refer to the Speciation Tool User Guide Appendix A for installation procedures of the required software.
```

Missing software/modules are indicated by a `[ ]` whereas modules/software that is installed and ready to be used are marked with `[x]`. Note that if PostgreSQL is erroneously shown as not installed, restarting the postgresql service can fix many of the reasons that might cause this to occur.

Perl

For the purposes of this guide, it is assumed that Perl has already been installed on your system. Almost every modern Linux distribution comes with Perl installed. To determine if Perl is installed, enter the following at the Linux command line:

```
# perl –v
```

If Perl is installed, information about the version will be displayed. Additional interfaces and modules for Perl need to be installed for the Speciation Tool to read text files and communicate with the database. Instructions for the installation of these modules follow the PostgreSQL installation section. PostgreSQL must be installed prior to installing the Perl database driver and interface.

PostgreSQL Installation

The Yum software package manager is an easy to use utility that installs, updates and removes software packages on RPM-based systems. This utility is found on RedHat, CentOS, Fedora, and other RPM-based Linux distributions. You can use yum to install PostgreSQL and the required Perl modules.

Note: For systems with different installation procedures/requirements, PostgreSQL pre-compiled binaries can be found at http://www.postgresql.org/. Click on the Downloads tab to review the available products. From http://www.postgresql.org/download/, choose the binary package corresponding to your operating system. As of writing, binary packages are available for the following operating systems:

- BSD
  - FreeBSD
  - OpenBSD
- Linux
  - RedHat/CentOS/Fedora/Scientific families Linux
  - Debian GNU/Linux
  - Ubuntu Linux
  - SuSE and OpenSuSE
  - Other Linux
- Mac OS X
- Solaris
- Windows

Install PostgreSQL using the Installation Wizard

To install PostreSQL using Yum, you will probably need to be logged in as root. To download and install PostgreSQL, execute the following command:

```
# yum install postgresql
```

If prompted, enter 'y' to confirm the installation. The package will download and install; additional packages may be automatically selected for install in order to resolve dependencies.

Install Perl database interface modules

Three Perl modules are required to read in text files and communicate with the database used by the Speciation Tool. They are:

Perl DBI (`perl-DBI`)	The Perl Database Interface allows communication between the Speciation Tool scripts and PostgreSQL database.
Perl DBD-Pg (or `perl-DBD-Pg`)	This is a PostgreSQL-specific database driver for the DBI module to allow Perl to communicate with the PostgreSQL database using the DBI.
or Perl DBD:PgPP	
Perl Text-CSV (`perl-Text-CSV`)	This module allows for Perl scripts to parse and create CSV (Comma Separated Values) files.

Use Yum to download and install (if needed) all three modules. Enter the command:

```
# yum install perl-DBI perl-DBD-Pg perl-Text-CSV
```

Enter 'y' when prompted to confirm the installation of these packages.

Note: If errors about packages not being found are displayed, check the spelling of the package names in your command; they are case-sensitive.

Start the PostgreSQL Service and Prepare It for the Speciation Tool

To start the PostgreSQL database service, execute the following command:

```
# /etc/init.d/postgresql start
```

Change to the user who will be running the Speciation Tool:

```
# su <user name here>
```

Start the terminal-based front-end to PostgreSQL (psql) with the default postgres user:

```
> psql –U postgres
```

Create PostgreSQL user(s) with database create option for each of the users that will be running the Speciation Tool. The user name should correspond to the Linux user account name. The command is:

```
=# CREATE USER <user name here> WITH CREATEDB;
```

Exit psql by entering "\q":

```
=# \q
```

At this point you should be ready to follow the Speciation Tool set up procedures (refer to Chapter 3). Run the script *sptool_reqd_checks.sh* to check that all of the packages are available to the Speciation Tool.

Windows Installation

This section provides the details for installing PostgreSQL and the Perl Database Interface (DBI, DBD:PgPP) in a Windows environment. Perl must be installed prior to PostgreSQL in order for the PostgreSQL Installation Wizard to offer the procedural language PL/perl.

Steps for Windows Installation:

1. Install Perl
2. Install PostgreSQL
3. Install additional Perl modules

Perl Installation

1. If necessary download ActivePerl software from http://www.activestate.com/
2. Unzip ActivePerl and click Installer.bat.
3. A DOS window will open, read and accept the license agreement.
4. Enter the top level directory for Perl installation.
5. Accept or decline Perl features by replying yes/no.
6. Proceed to start the installation.
7. Restart your computer before you proceed with the PostgreSQL installation.

PostgreSQL Installation

PostgreSQL can be found at http://www.postgresql.org/. Click on the Downloads tab to review the products available. From http://www.postgresql.org/download/ click FTP Browser followed by selecting the win32 subdirectory. From this subdirectory download postgresql-8.1.4-1.zip.

Prior to installing PostgreSQL

Check the file system of the hard drive on which PostgreSQL will be installed. The NTFS file system has a comprehensive access control system and offers the reparse point functionality to implement tablespaces used by PostgreSQL. The PostgreSQL installer package will not initialize a database cluster on anything but an NTFS partition. FAT and FAT32 file systems do not offer such reliability. It is necessary that a FAT or FAT32 disk be converted to NTFS prior to installation of PostgreSQL.

To determine the file system of the hard drive, through Windows Explorer, highlight the drive, right click and select Properties. The General tab of the Local Disk Properties window displays the current file system of the selected drive.

To convert FAT/FAT32 to NTFS:

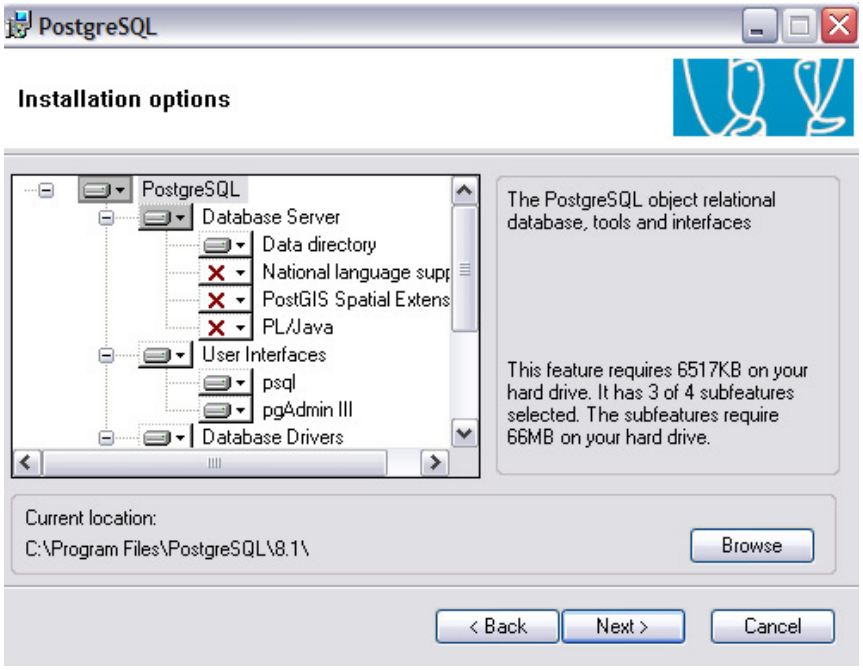
1. open a DOS window
2. from the DOS command prompt enter the command
   convert drive_letter: /fs:ntfs.

For example, typing convert D: /fs:ntfs would format the D: drive to the ntfs file system format. It is a good practice to backup all important data prior to the conversion.

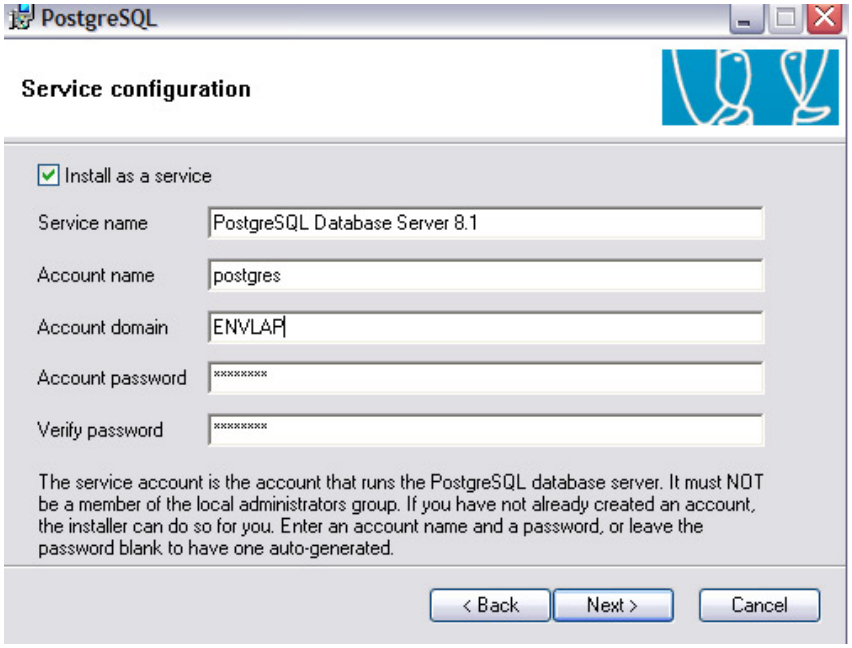
Install PostgreSQL using the Installation Wizard

A complete description of the installation process can be found at http://pginstaller.projects.postgresql.org/ (accessed on 09/21/2006).

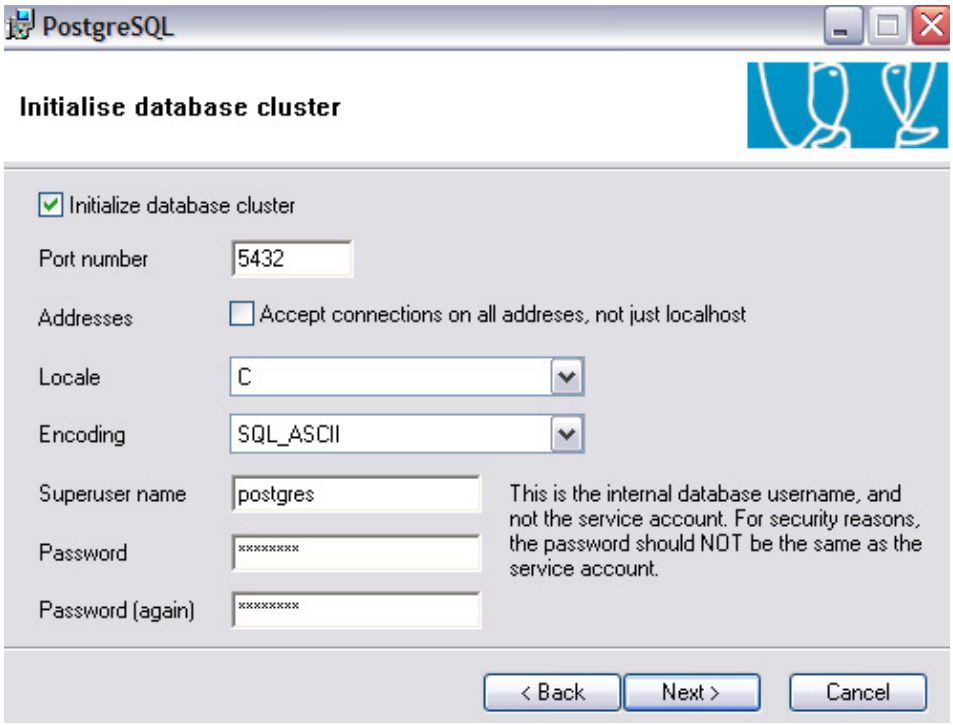
1. Unzip the PostgreSQL software that you downloaded.
2. Execute (double-click on) postgresql-8.1.msi. This will start the installation wizard.
3. Select the language you want to use for the installer and click Start.
4. Click Next to continue the installation following the Welcome message.
5. Click Next to continue following the Installation notes.
6. In the Installation options window, verify that "Database Server" > "Data directory", "User Interfaces", and "Database drivers" are selected. You may change the PostgreSQL installation directory by clicking on Browse and specifying the directory of your choice.



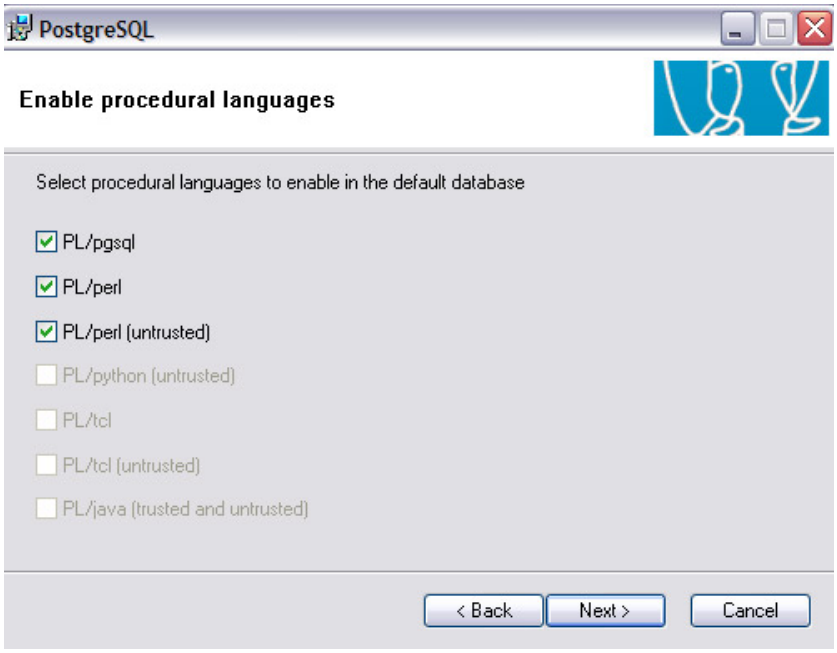
7. In the Service configuration window install PostgreSQL as a service by checking the box "Install as a service". Provide and verify a password for the account name "postgres". This is only for an administrator to run the PostgreSQL database server. Click Next to continue. Click Yes if you get the error message "Would you like the account to be created for you?"



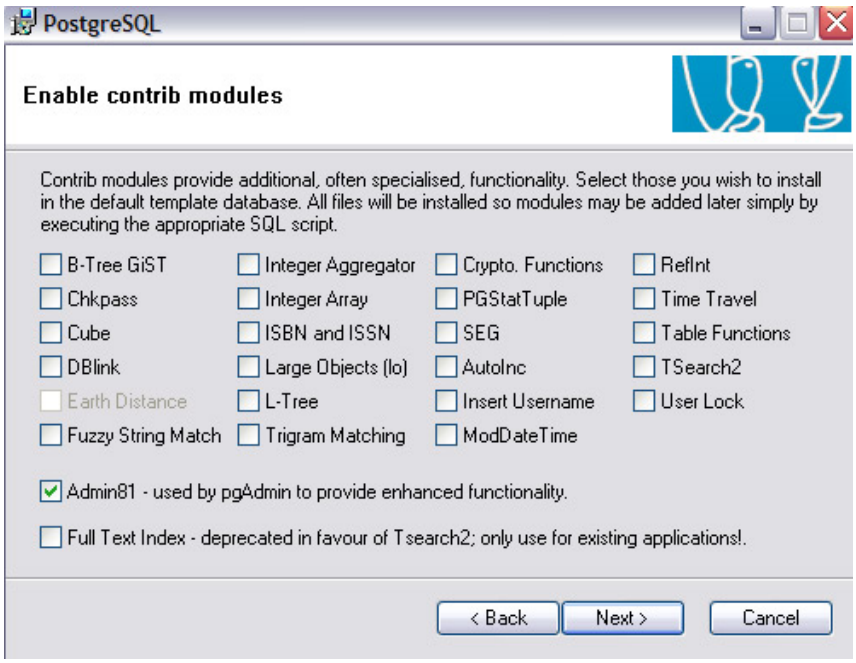
8. In the Initialize database cluster window provide the superuser name postgres and a password. Click Next to continue.



9. In the Enable procedural languages window select PL/pgsql, PL/perl and PL/perl (untrusted) to be enabled in the default database. Click Next to continue.



10. Click Next to use the default setting of Admin81.



11. Click Next to start the actual installation .

Please note that these steps are applicable to PostgreSQL version 8.1. Consult the PostgreSQL website if installing a later version.

PostgreSQL Client Authentication

PostgreSQL offers a number of different client authentication methods. The method used to authenticate a particular client connection can be selected on the basis of (client) host address, database, and user. The Speciation-PC Tool is set to trust users by running on the local host without a password. To allow this setting in PostgreSQL, users will have to modify a client authentication setting. The client authentication is controlled by a configuration file, which traditionally is named pg_hba.conf and is stored in the database's data directory; i.e. C:\Program Files\PostgreSQL\8.1\data.

To change the client authentication

1. Open pg_hba.conf file (text format) in the database's directory.
2. Modify the configuration file by adding a "trust" entry in "METHOD" field and save.

```
#TYPE  DATABASE    USER        CIDR-ADDRESS          METHOD
host    all         all         127.0.0.1/32          trust
```

3. If this step is done after PostgreSQL service is running, stop the service, reload configuration and restart the service (Click Start Menu>Programs>PostgreSQL 8.1> Stop service, Reload configuration, Start service). Otherwise, only click reload configuration.

Install Perl database interface Modules

The following procedures, utilizing the PPM, require a connection to the internet. Alternatively, these packages can be downloaded manually and loaded offline.

1. Open a DOS window and start Perl's Programmer's Package Manager by entering "ppm" on the command line.
2. At the ppm command prompt, install DBI by entering "install DBI".
3. At the ppm command prompt, install DBD:PgPP by typing "install DBD-PgPP".
4. At the ppm command prompt, install Text-CSV by typing "install Text-CSV".

At this point, if all directions have been followed without error, you should be ready to follow the Speciation Tool set up procedures.

APPENDIX B

SHARED Schema File Formats

A field name in blue indicates an indexed field.

Table B1. tbl_carbons.

Field Name	Field Type	Description
mechanism	Character 20	Mechanism name
aqm_poll	Character 20	Air quality model lumped species identifier/name
num_carbons	Numeric (5,2)	Number of carbon bonds for lumped species

Table B2. tbl_gas_profile_weights.

Field Name	Field Type	Description
profile_id	Character 20	Profile identifier
specie_id	Character 20	Unique species identifier
percent	Numeric (10,6)	Percentage of pollutant in profile
uncertainty	Numeric (10,6)	Uncertainty percent of pollutant
unc_method	Character 100	Description of method used to determine uncertainty
analytic_method	Character 500	Description of analytical method

Table B3. tbl_gas_profiles.

Field Name	Field Type	Description
profile_id	Character 20	Unique profile identifier
profile_name	Character 200	Profile name
quality	Character 10	Overall Quality Rating
controls	Character 100	Emission controls
date_added	Date	Date profile added
notes	Character	Notes
total	Numeric (10,5)	Sum of profile percentages
master_poll	Character 20	Basis of profile
test_method	Character	Test method description
norm_basis	Character 100	Normalization description
composite	Character 1	Indicates if profile is original or composite; O or C
standard	Boolean	Standard or user added profile
test_year	Character 50	Year testing was completed
j_rating	Numeric (10,2)	Judgment rating based on general merit
v_rating	Numeric (10,2)	Vintage Rating
d_rating	Numeric (10,2)	Data quality rating based on number of observations
region	Character 100	Geographic region of relevance
old_profile	Integer	Profiles taken from previous version
sibling	Character 20	Profile_ID of PM profile from same study
voc_to_tog	Numeric (12,7)	VOC to TOG conversion factor
data_origin	Character 50	Originating organization
primary_prof	Boolean	
description	Character	Profile description
documentation	Character	Documentation of profile origin

Table B4. tbl_invtable.

Field Name	Field Type	Description
eminv_poll	Character 12	Emission inventory pollutant name
mode	Character 3	Process mode
poll_code	Character 16	Pollutant code
specie_id	Character 20	Species identifier
reactivity	Character 20	Reactivity group
keep	Character 20	Keep flag; Y or N
factor	Character 20	Adjustment factor
voc	Character 20	VOC or TOG component flag
model	Character 20	Model species flag
explicit	Character 20	Explicit in mechanism flag
activity	Character 20	Data type flag; Y indicates activity (not emissions)
nti	Character 20	Identifies HAPs on the Clean Air List
unit	Character 20	Units
description	Character 50	Inventory data description
cas_description	Character 50	CAS pollutant description

Table B5. tbl_mechanism.

Field Name	Field Type	Description
mechanism	Character 20	Mechanism name
specie_id	Character 20	Unique species identifier
aqm_poll	Character 20	Air Quality Modeling lumped pollutant identifier
moles_per_mole	Numeric (20,12)	The moles per mole

Table B6. tbl_mechanism_description.

Field Name	Field Type	Description
mechanism	Character 20	Mechanism name
description	Character 256	Description
nonsoaflag	Character 1	Flag: "N" SOA mechanism "Y" nonSOA mechanism
origin	Character 300	Originating organization
reference	Character 100	References
comment	Character 500	Comment

Table B7. tbl_metadata.

Field Name	Field Type	Description
keyword	Character 20	Metadata keyword
dativa l	Character 256	Corresponding value (file)
version	Character 20	Data version

Table B8. tbl_pm_mechanism.

Field Name	Field Type	Description
mechanism	Character 20	Mechanism name
specie_id	Character 20	Unique species identifier
aqm_poll	Character 20	Air Quality Modeling lumped pollutant identifier
qualify	Boolean	Indicates which species determines if a profile qualifies for the specified mechanism
compute	Boolean	If true, compute aqm_poll (usually PMFINE or PMOTHR)

Table B9. tbl_pm_profiles.

Field Name	Field Type	Description
profile_id	Character 20	Unique profile identifier
profile_name	Character 255	Profile name
quality	Character 10	Overall Quality Rating
controls	Character 150	Emission controls
date_added	Date	Date profile added
notes	Character	Notes
total	Numeric (10,5)	Sum of profile percentages
master_poll	Character 20	Basis of profile
test_method	Character	Test method description
norm_basis	Character 100	Normalization description
composite	Character 1	Indicates if profile is original or composite; O or C
standard	Boolean	Standard or user added profile
incl_gas	Boolean	
test_year	Character 50	Year testing was completed
j_rating	Numeric (10,2)	Judgment rating based on general merit
v_rating	Numeric (10,2)	Vintage Rating
d_rating	Numeric (10,2)	Data quality rating based on number of observations
region	Character 100	Geographic region of relevance
lower_size	Numeric (10,4)	
upper_size	Numeric (10,4)	
sibling	Character 20	Profile_ID of PM profile from same study
data_origin	Character 50	Originating organization
primary_prof	Boolean	
description	Character	Profile description
documentation	Character	Documentation of profile origin

Table B10. tbl_pm_profile_weights.

Field Name	Field Type	Description
profile_id	Character 20	Profile identifier
specie_id	Character 20	Unique species identifier
percent	Numeric (12,6)	Percentage of pollutant in profile
uncertainty	Numeric (12,6)	Uncertainty percent of pollutant
unc_method	Character 100	Description of method used to determine uncertainty
analytic_method	Character 500	Description of analytical method

Table B11. tbl_rename_species

Field Name	Field Type	Description
aq_model	Character 10	AQM Model
mechanism	Character 20	Mechanism name
eminv_poll	Character 20	Compound name
aqm_poll	Character 20	Replacement AQM compound name

Table B12. tbl_species.

Field Name	Field Type	Description
specie_id	Character 20	Unique species identifier
specie_name	Character 100	Species name
CAS	Character 50	CAS identifier
epaid	Character 50	EPA identifier
saroad	Character 10	Old SAROAD code
pams	Boolean	Yes or No to PAMS
haps	Boolean	Yes or No to HAPs
symbol	Character 10	Symbolic name
molecular_weight	Numeric (20,12)	Molecular weight of specie
non_voctog	Boolean	Yes or No to non-volatile organic gas
non_vol_wt	Character 20	Non-volatile weight
unknown_wt	Character 20	Unknown weight
unassign_wt	Character 20	Unassigned weight
exempt_wt	Character 20	Exempt weight
volatile_mw	Numeric (20,12)	Volatile molecular weight
num_carbons	Numeric (20,12)	Number of carbon bonds
epa_itn	Character 20	EPA internal tracking number
comment	Character 50	Comments

Table B13. tbl_static.

Field Name	Field Type	Description
profile_id	Character 20	Profile identifier
eminv_poll	Character 20	Emission inventory pollutant code
aqm_poll	Character 20	AQM species code
split_factor	Numeric (20,10)	Mole based split factor (numerator)
divisor	Numeric (20,10)	Denominator of the mole based factor
mass_fraction	Numeric (20,10)	Mass fraction
aq_model	Character 10	Air Quality Model

Table B14. tbl_camx_fcrs.

Field Name	Field Type	Description
profile_id	Character 20	Profile identifier

Table B15. tbl_vbs_ivoc_nmogfactors.

Field Name	Field Type	Description
profile_id	Character 20	Profile identifier
cmaq_ivocname	Character 20	CMAQ IVOC compound name
camx_ivocname	Character 20	CAMx IVOC compound name
nmogfraction	Numeric (10,6)	Fraction of NMOG assigned to IVOC compounds

Table B16. tbl_vbs_ivoc_species.

Field Name	Field Type	Description
aqm	Character 20	Air Quality Model name
specie_id	Character 20	IVOC compound name (assigned in Table B15)
molwt	Numeric (10,6)	Molecular weight of IVOC compound

Table B17. tbl_vbs_svoc_factors.

Field Name	Field Type	Description
profile_id	Character 20	Profile identifier
cmaq_svocname	Character 20	CMAQ SVOC compound name
camx_svocname	Character 20	CAMx SVOC compound name
bin0	Numeric (10,6)	Fraction of POA assigned to SVOC_bin0
bin1	Numeric (10,6)	Fraction of POA assigned to SVOC_bin1
bin2	Numeric (10,6)	Fraction of POA assigned to SVOC_bin2
bin3	Numeric (10,6)	Fraction of POA assigned to SVOC_bin3
bin4	Numeric (10,6)	Fraction of POA assigned to SVOC_bin4

APPENDIX C

RUN Schema File Formats

Table C1. tbl_gas_process.

Field Name	Field Type	Description
profile_id	Character 20	Profile identifier
process	Character 20	Process mode

Table C2. tbl_primary.

Field Name	Field Type	Description
aqminv_poll	Character 20	Inventory pollutant name
aqm_add	Character 20	Compound name to add
split_factor	Numeric (12,8)	Split factor for added compound
writeflag	Character 1	Flag: "N" – compound should be added "Y" – compound should be replaced

Table C3. tbl_run_control.

Field Name	Field Type	Description
keyword	Character 20	Key word identifying function or file name
datival	Character	Corresponding value for the key word

Table C4. tbl_toxics.

Field Name	Field Type	Description
aqm_model	Character 20	AQM name
specie_id	Character 20	Unique species identifier
aqm_poll	Character20	Air quality model lumped species identifier/name
num_carbons*	Numeric (6,3)	Number of carbon bonds for lumped AQM pollutant
active*	Character 1	Options: A – active, T - tracer

* Not a user input; assigned by the system.

Table C5. tbl_user_profile_wts.

Field Name	Field Type	Description
profile_id	Character 20	Profile identifier
specie_id	Character 20	Unique species identifier
percent	Numeric (10,6)	Percentage of pollutant in profile

Table C6. Table names in the run schema created by the Speciation Tool for internal calculations.

Table Name	Description
tmp_actox	Checks for profiles with 100% active toxics.
tmp_aqm_carbons	Initialized with shared .tbl_carbons. Records are added for user specified toxic species.
tmp_calcs_byaqm	Store intermediate calculations by mechanism, profileId, and AQM pollutant. Includes moles per gram, moles model species per mole emissions, and average molecular weight .
tmp_calcs_byspc	Stores intermediate calculations by mechanism, profileId, specieId, and AQM pollutant. Includes moles per gram, moles model species per mole emissions, mole weight percent of model species, grams per mole, and average molecular weight.
tmp_calcs_haps	Store intermediate calculations by mechanism, profileId, specieId, emission inventory pollutant, and AQM pollutant for the user specified HAPs species. Includes moles per mole, moles per gram, and average molecular weight.
tmp_calcs_haps_null	Stores the calculated average molecular weights for those records in tmp_calcs_haps with undefined average molecular weights.
tmp_camxpm_splits	Stores PM split factors for CAMx AQM
tmp_error	Stores run error messages.
tmp_gscnv	Stores the output converserion factor data.
tmp_gspro	Stores the output splits factor data.
tmp_haps	Stores the list of HAPs extracted from the INVTABLE.
tmp_header	Stores the NONHAPTOG header entries.
tmp_invtable	Used for checking output pollutant name widths specified in INVTABLE.
tmp_mechanism	Initialized with the user selected mechanism from shared tbl_mechanism or tbl_pm_mechanism. Records are removed or inserted depending on run parameters.
tmp_metadataset	Stores the metadata written to the header of the output files.
tmp_prfwts	Stores the
tmp_pm_mechanism	Mechanism definition for user specified PM mechanism run
tmp_pm_splits	$PM_{2.5}$ split factors
tmp_prfwts	Initialized with tmp_raw_profiles. Data records are removed and renormalized depending upon run parameters.
tmp_profile_list	Stores the unique list of PM profiles
tmp_qa_carbons	Stores AQM compounds where no carbon data has been specified.
tmp_qa_mechanism	Stores species with no corresponding mechanism definition.
tmp_raw_profiles	Initialized with either shared .tbl_gas_profile_weights, tbl_pm_profile_weights, or tbl_user_profile_wts if user provided.
tmp_species	Stores the verified species list
tmp_species_carbons	Stores the calculated number of carbons for each species.
tmp_spcinp	Stores user specified species that have invalid molecular weights.
tmp_sumnmog	Stores the sums of NMOG components
tmp_sums	Stores the profile weights percent sums during renormalization.
tmp_vbs_svoc_factors	Stores the SVOC factors for VBS processing
tmp2_qa_mechanism	Stores species for selected profiles with no mechanism definition.

APPENDIX D

PM2.5 Chemical Mechanism Definitions

Table D1 represents the AE5 and AE6 chemical mechanism definitions. Table D2, prepared by EPA, provided the information used to define Table D1.

Table D1. Chemical Mechanisms AE5 and AE6 as input to the Speciation Tool.

Chemical Mechanism	SpecieID	AQM Pollutant	Qualify	Compute
AE5				
AE5	626	POC	T	F
AE5	797	PEC	T	F
AE5	699	PSO4	T	F
AE5	613	PNO3	T	F
AE5		PMFINE	F	T
AE6				
AE6	626	POC	F	F
AE6	797	PEC	F	F
AE6	699	PSO4	F	F
AE6	613	PNO3	F	F
AE6	784	PNH4	F	F
AE6	2669	PNCOM	T	F
AE6	488	PFE	F	F
AE6	292	PAL	F	F
AE6	694	PSI	F	F
AE6	715	PTI	F	F
AE6	329	PCA	F	F
AE6	525	PMG	F	F
AE6	669	PK	F	F
AE6	526	PMN	F	F
AE6	696	PNA	F	F
AE6	795	PCL	F	F
AE6	2668	PH2O	T	F
AE6		PMOTHR	F	T

Table D2. Chemical Mechanisms AE5 and AE6 as defined by EPA

SPECIATE speciesID	Species Description	Species Name	Calculation	Notes
	CMAQ AE5:			
626	organic carbon	POC	explicit	measured
797	elemental carbon	PEC	explicit	measured
699	sulfate	PSO4	explicit	measured
613	nitrate	PNO3	explicit	measured
	unspeciated $PM_{2.5}$	PMFINE	1-(sum of 4 species)	n/a
	CMAQ AE6:			
626	organic carbon	POC	explicit	measured
797	elemental carbon	PEC	explicit	measured
699	sulfate	PSO4	explicit	measured
613	nitrate	PNO3	explicit	measured
784	ammonium	PNH4	explicit in 911XX profiles	measured
2669	non-carbon organic matter	PNCOM	explicit in 911XX profiles	PNCOM = POC*(OM/OC Ratio - 1) where OM/OC ratio is 1.25 for motor vehicle exhaust, 1.7 for wood combustion, 1.4 for other sources.
488	iron	PFE	explicit in 911XX profiles	measured
292	aluminum	PAL	explicit in 911XX profiles	measured
694	silica	PSI	explicit in 911XX profiles	measured
715	titanium	PTI	explicit in 911XX profiles	measured
329	calcium	PCA	explicit in 911XX profiles	measured
525	magnesium	PMG	explicit in 911XX profiles	measured
669	potassium	PK	explicit in 911XX profiles	measured
526	manganese	PMN	explicit in 911XX profiles	measured
696	sodium	PNA	explicit in 911XX profiles	measured
795	chloride	PCL	explicit in 911XX profiles	measured
2668	water	PH2O	explicit in 911XX profiles	0.24*(PNH4+PSO4) for non-combustion sources, 0 for combustion sources or use measured value of hydrated water, if available
	unspeciated $PM_{2.5}$	PMOTHR	1 - (sum of 17 species)	n/a

* A note on chloride from M. Strum (EPA OAQPS): only species 795 (chlorine atom) is used to populate PCL rather than using species 337 (chloride ion) or using both 795 and 337 because in the current $PM_{2.5}$ profiles in SPECIATE 4.3 when chloride (species 337) is present species 795 (chlorine atom) is also present. Including both of these would be double counting. In addition, per communication with Adam Reff (email from Adam Reff to Madeleine Strum, 3/24/2011), Reff indicates that chlorine atom (via XRF) is a more complete representation of all forms of Cl that might be present.