

7.0 CONCEPT Speciation Profile Development Model**Table of Contents**

- 7.1 Overview
- 7.2 Functionality
 - 7.2.1 Input and QA foundation data in RPO formats
 - 7.2.2 Calculate Lumped Profile
- 7.3 Control Variables Options
- 7.4 Input File Structures
- 7.5 Lookup and Cross-reference File Requirements
 - 7.5.1 Data Validation Lookup Tables
- 7.6 Intermediate and Temporary Tables
- 7.7 Report Options
 - 7.7.1 Input Data QA Results

List of Figures and Tables

- Figure 7.3.1 CONCEPT Speciation Profile Development
- Table 2.3.1 Run control variables affecting the Speciation Profile Development model
- Table 7.4.1 Speciation Profile Development input file requirements.
- Tables 7.4.2 – 2.4.4 contain the structural elements of the required RPO input files.
- Table 7.4.2 Speciation Compound List (rpo_cl.txt)
- Table 7.4.3 Speciation Profile (rpo_sp.txt)
- Table 7.4.4 Speciation Compound Assignment (rpo_ca.txt)
- Table 7.6.1 Intermediate Tables Produced for Speciation Profile Development
- Table 7.7.1 Speciation Profile Development QA Result Reports

7.1 Overview

The purpose of the speciation model is to create updated speciation factors from foundation chemical speciation data, such as SPECIATE. The lumped profiles for CB-IV, SAPRC or PM species may be created, providing the underlying data is adequate. The speciation model does extensive QA on the input data, and provides summaries and feedback to evaluate the adequacy of the revised profiles.

The user will provide to the model:

- Compound List (rpo_cl format)
- Compound Assignments (rpo_ca format)
- Speciation Profiles (not lumped profiles, rpo_sp format)

To run the speciate model, the CONCEPT system must be initialized, and the global and xref files loaded into the database (See section 1.6 Setting up a project)

The concept script commands to run the speciation model is:

```
concept build_speciation -n PROJECTNAME -s SCENARIO_NAME -d DIRECTORY [-t]
```

Where -d indicates the location of the input files to be used in creating the new spatial allocation factors. The CONCEPT distribution contains, in the concept directory, an example script (speciate_beta4.sh) that runs the speciation model for project = beta4, scenario = scenario1, input data located at concept_projects/beta4/speciate/Ladco_update.

7.2 Functionality

To produce the lumped speciation profiles from the foundation chemical speciation data, the Speciation Profile Development model performs three distinct functions. These steps are incorporated into the concept script command.

1. Input and QA foundation data in RPO formats.
2. Calculate revised lumped profile
3. Output the revised lumped profiles into the rpo_lp format.

7.2.1 Input and QA foundation data in RPO formats

Data to create new or updated speciation profiles must be supplied to CONCEPT via the RPO formats for Compound List (rpo_cl), Compound Assignment (rpo_ca) and Speciation Profile (rpo_sp, these are the pre-lumped profiles using the detailed compounds rather than the lumped compound groups)

These file are input and selected fields are reviewed are completeness:

- A) Chemical IDs cannot be blank.

- B) Chemical Mechanisms must match between the input files and the CONCEPT scenario run_control file.
- C) Molecular Weights must exist and be > 0.

7.2.2 Calculate Lumped Profile

- A. Summarize the mass fractions in rpo_sp by lumped compound group and profile.
- B. Calculate split factor as:
$$\text{split_factor} = (\text{mass_fraction}/\text{molecular_weight}) * \text{mole_factor}$$

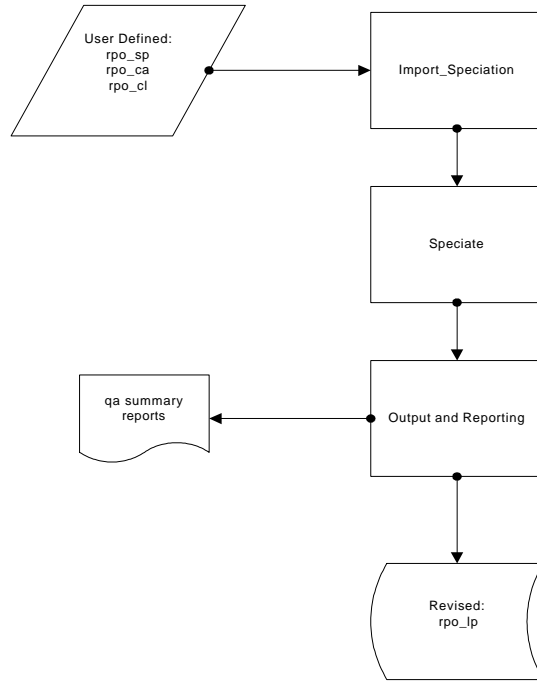
Where mass_fraction is calculated from rpo_sp
molecular_weight is from rpo_cl
mole_factor is from rpo_ca

7.2.3 Output the revised profiles in rpo_lp format.

The calculated speciation profiles are stored in the rpo_lp sql data table. The rpo_lp table will be replaced entirely, not updated. These profiles are also written to an external file, located in the directory designated in the concept script command (IE. concept build_speciation -n beta4 -s scenario1 -d concept_projects/beta4/speciate/Ladco_update) The output file is name rpo_lp.calc and can be used to update the rpo_lp.txt ASCII file.

Figure 7.3.1

CONCEPT SPECIATION PROFILE DEVELOPMENT



7.3 Control Variables Options

The run control text file is located in the concept_projects/project_name/scenario_name directory. Each run_control file is specific to the modeling scenario, with each scenario specific to the modeling grid, episode dates, and chemical mechanism.

Table 7.3.1 Run control variables affecting the Speciation Profile Development model

Variable Name	Description	Valid Options
ChemicalMechanism	Mechanism for speciation	CBIV, SAPRC

7.4 Input File Structures

Input data to the Speciation Profile Development Model is based on the RPO data exchange structures. The model requires 3 input files, as well as the existing speciation file as read in during the project set-up routines.

Table 7.4.1 Speciation Profile Development input file requirements.

NEI File Name	CONCEPT Reference Name		Input File Location
SpeciateSP	rpo_sp	required	Designated by -d option in script
SpeciateCA	rpo_ca	required	Designated by -d option in script
SpeciateCL	rpo_cl	required	Designated by -d option in script

Tables 7.4.2 – 2.4.4 contain the structural elements of the required RPO input files.

Table 7.4.2 Speciation Compound List (rpo_cl.txt)

Field Name	Description	Type	Size	Begin	End
RECORD_TYPE	A code that identifies the type of record (CL)	CHARACTER	2	1	2
CHEMICAL_ID	Chemical Compound ID	CHARACTER	15	3	17
CHEMICAL_ABBREC	Chemical compound abbreviation	CHARACTER	9	18	26
CHEMICAL_NAME	Chemical compound name	CHARACTER	80	27	106
CARBON_NUMBER	Number of carbon atoms	NUMBER	20	107	126
MOLE_WEIGHT	Molecular weight	NUMBER	20	127	146

Table 7.4.3 Speciation Profile (rpo_sp.txt)

Field Name	Description	Type	Size	Begin	End
RECORD_TYPE	A code that identifies the type of record (SP)	CHARACTER	2	1	2
POLLUTANT_CODE	Pollutant ID	CHARACTER	9	3	11
PROFILE_CODE	Individual speciation profile code	CHARACTER	15	12	26
CHEMICAL_ID	Chemical compound ID	CHARACTER	15	27	41
MASS_FRACTION	Mass Fraction	NUMBER	10	42	51

Table 7.4.4 Speciation Compound Assignment (rpo_ca.txt)

Field Name	Description	Type	Size	Begin	End
RECORD_TYPE	A code that identifies the type of record (CA)	CHARACTER	2	1	2
CHEMICAL_MECHANISM	Chemical mechanism code (indicate degree of lumping if variable, as is the case for SAPRC-99)	CHARACTER	10	18	27
CHEMICAL_ID	Pollutant id	CHARACTER	9	28	36
MOLE_FACTOR	Chemical Mechanism Group	CHARACTER	10	37	46
CHEM_MECH_GROUP	Divisor	NUMBER	10	47	56
SPLIT_FACTOR	Model chemical compound name used to represent the compound name	NUMBER	10	57	66

7.5 Lookup and Cross-reference File Requirements

The Spatial Profile Development Model does not require any of the lookup and cross-reference tables utilized by other modules of CONCEPT. The output of the Spatial Profile Development Model is an updated version of the rpo_lp table. The model produces both an updated POSTGRES data table, and an updated ASCII (rpo_lp.calc) file for archival purposes. Note that this model creates a new rpo_lp table, rather than updating any versions that may already exist for the project.

7.5.1 Data Validation Lookup Tables

The Speciation Profile Development Model does not require any of the Data Validation Lookup tables used by other CONCEPT modules. The Model does run QA steps on the input speciation data files for the following fields:

- A) Chemical IDs cannot be blank.
- B) Chemical Mechanisms must match between the input files and the CONCEPT scenario run_control file.
- C) Molecular Weights must exist and be > 0.

7.6 Intermediate and Temporary Tables

The Speciation Profile Development Model produces a number of intermediate data tables that may be of interest to the user for data review and QA. The structure of these tables can easily be reviewed using the POSTGRES display table command (`\d tablename`).

Table 7.6.1 Intermediate Tables Produced for Speciation Profile Development

Created By	Table Name	Description
speciate.sql	qa_spec_sp	Speciation Profile (SP) records with no chemical ID
speciate.sql	qa_spec_mf	Speciation Profile (SP) summary of mass fraction by pollutant
speciate.sql	qa_spec_ca	Chemical Assignment (CA) records with no chemical ID
speciate.sql	qa_spec_cl_cas	Chemical List (CL) records with no chemical ID
speciate.sql	qa_spec_cl_mw	Chemical List (CL) records with missing molecular weights
speciate.sql	voc_rpo_lp	Calculated lumped profiles for VOC species only
speciate.sql	non_von_rpo_lp	Calculated lumped profiles for PM species only

7.7 Report Options

The CONCEPT speciation profile development model produces two QA reports and an ASCII copy of the revised rpo_lp file (rpo_lp.calc). The output reports and updated file will be located in the directory identified in the CONCEPT script call as the location for the input chemical data:

```
concept build_speciate -n beta4 -s scenario1 -d ../concept_projects/beta4/scenario1/Ladco_update
```

7.7.1 Input Data QA Results

These reports summarize the input records that are affected by missing or default data. Currently included in the reports are the results of QA procedures performed on the Chemical Assignment (rpo_ca) and Speciation Profile (rpo_sp) input file. Two QA reports are produced:

Table 7.7.1 Speciation Profile Development QA Result Reports

Report Name	Description
speciation_ca_qa_report	Chemical Assignment records with missing chemical IDs
speciation_sp_qa_report	Speciation Profiles with missing fraction (% of profile unaccounted for)