Instructions for Speciating MOVES Emissions

Introduction

This document provides instructions for using the post-processing scripts that calculate speciation profile weights used to speciate residual total organic gases (NONHAPTOG), particulate matter (PM), total organic matter (TOM), and residual particulate matter (nonSO4nonECnonOM) for MOVES4 and later versions. This step is needed only in cases where the user needs to convert these emissions into chemical mechanism species for use in air quality models. These scripts are designed in particular for users interested in running the Sparse Matrix Operator Kernel Emissions (SMOKE) modeling system[i] and include SMOKE Source Classification Codes (SCC) in the output.

Speciation is the process of allocating organic aggregate species to chemical mechanism and/or real species. This is done using speciation profiles stored in EPA's SPECIATE database.[ii] MOVES calculates emissions for some organic gas (onroad and nonroad) and PM (onroad only) species directly, often because MOVES applies adjustments for temperature and fuels that depend on vehicle technology. These pollutants are referred to as "integrated species" that contribute to both total organic gases (TOG) and particulate matter ($PM_{2.5}$). The list of specific species is detailed in the technical reports Speciation of Total organic Gas and Particulate Matter in MOVES4 (EPA-420-R-23-006) and Speciation Profiles and Toxic Emissions for Nonroad Engines in MOVES4 (EPA-420-R-23-013).

The mass of TOG or PM left to be speciated after subtracting out integrated species is called residual TOG (NONHAPTOG) and residual PM (NonECNonSO4NonOM PM). PM organic matter and total PM from nonroad can also be speciated by post-processing emissions with these scripts.

Speciation Profiles

MOVES4 supports two sets of speciation profiles. The first set of profiles are consistent with chemical mechanisms supported in previous versions of MOVES, such as CB5 and CB6. In the GUI, these profiles are referred to as the "Non-volatility resolved" speciation profile set. The scripts also provide updated speciation profiles and a ratio that can be used to calculate Condensable and Gaseous Reactive Organic Carbon (CROC and GROC, respectively) to support speciation using the new "Reactive Organic Carbon" (ROC) framework.[iii] Finally, the scripts also handle the conversion from MOVES SCC output into SMOKE SCC format.

Speciation profiles are assigned to specific onroad sources depending on fuel type, fuel subtype, model year, regulatory class, and emission process. The mapping of each of these parameters to SPECIATE profiles is detailed in the rocSpeciation table of the MOVES default database. The post-processing script uses this table to assign speciation profiles to each Source Classification Code (SCC). In some cases, a given SCC is assigned more than one speciation profile because SCCs are defined at the source type level, whereas speciation profiles are also defined by model year and fuel subtype. In this case, the "profileContribution" field describes the fraction of the SCC emissions associated with the listed profile. The profileContributions sum to one for each SCC. A profileContribution of one indicates that the SCC is represented by a single profile.

Speciation profiles are assigned to specific nonroad sources depending on fuel type, fuel subtype, engine technology including tier and strokes, and emission process. The mapping by each of these parameters to SPECIATE profiles is detailed in the nrROCSpeciation table of the MOVES default database. The post-processing scripts match MOVES nonroad output to the appropriate speciation profile.

Instructions

The speciation scripts can be run from the Speciation Profile Scripts tool, available in the Tools menu of the MOVES GUI, once users have completed the required MOVES runs. The following sections for onroad and nonroad detail the conditions that need to be met for the scripts to run and perform as intended.

Onroad

For the onroad post-processing script to run, the following conditions need to be met:

- The MOVES run output must have the relevant pollutants to be speciated (NONHAPTOG, nonSO4nonECnonOM, and TOM). These are selected in the RunSpec via the Pollutants and Processes panel, along with all prerequisites.
- The MOVES run output must provide detail by SCC, source type, fuel type, model year, emission process, regulatory class, and road type. These are selected in the RunSpec via the Output Emissions Detail Panel of the GUI.
- The MOVES output database containing emissions to be speciated may contain multiple MOVES runs but must only contain output for a single calendar year. Multiple counties are allowed.

The output of the script is a series of tables that list the fraction of residual TOG, residual PM, and TOM emissions that should be speciated with the given profile (as well as the CROC and GROC ratios if the Reactive Organic Carbon profile set is selected) saved into the database specified by the user.

Steps to run the Onroad Speciation Profile Weighting Scripts

1. Open MOVES and perform the MOVES runs that will generate the output to be speciated, following the instructions above to make sure the appropriate emissions detail is available in the output database.
2. Open the Speciation Profile Scripts from the MOVES Tools menu.
3. Ensure that “Onroad” is the selected model and select the desired profile set.
4. Select the MOVES output database from Step 1 in the Output Database dropdown menu.
5. Select the desired database to hold the script output. An existing database can be used or a new one can be specified, depending on user preference.
6. Click “Run Profile Weighting Script”. Depending on the nature of the run, it may take a couple minutes to complete.

Nonroad

For the nonroad post-processing script to run, the following conditions need to be met:

- The MOVES run output must have the relevant pollutants to be speciated (NONHAPTOG and $PM_{2.5}$) selected via the Pollutants and Processes panel, along with all prerequisites.
- The MOVES run output must provide detail by SCC, fuel type, fuel subtype, engine tech, and emission process. These are selected in the RunSpec on the Output Emissions Detail Panel.
- The MOVES output database containing emissions to be speciated may contain multiple MOVES runs but must only contain output for a single calendar year. Multiple counties are allowed.

The output of the script is a pair of tables that list the speciation profiles and ratios used for residual TOG and $PM_{2.5}$, saved into the database specified by the user.

Steps to run the Nonroad Speciation Profile Script

1. Open MOVES and perform the MOVES runs that will generate the output to be speciated, following the instructions above to make sure the appropriate emissions detail is available in the output database.
2. Open the Speciation Profile Scripts from the MOVES Tools menu.
3. Ensure that "Nonroad" is the selected model and select the desired profile set.
4. Select the MOVES output database from Step 1 in the Output Database dropdown menu.
5. Select the desired "New Database" to hold the script output. An existing database can be used or a new one can be specified, depending on user preference
6. Click "Run Profile Weighting Script". Depending on the nature of the run, it may take a couple minutes to complete.

Script Outputs

The scripts output tables which map MOVES emissions to speciation profiles. These are saved in the database selected by the user. If the Reactive Organic Carbon profile set is selected, ratios are provided to calculate CROC and GROC from the MOVES output, as well as residual PM.

Onroad

The onroad scripts output four tables for NONHAPTOG speciated emissions output: exhaust (exh_groc), evaporative (evp_groc), evaporative permeation (epm_groc), and refueling (rfl_groc). For speciation of total organic matter (which is used to calculate CROC) or residual PM, the SQL output database contains a single table for exhaust emissions (exh_croc or exh_residpm). The SQL output database also contains an ancillary table that describes the mapping between MOVES emission processes and SMOKE processes.

Each output table follows the same general schema as described in the following table.

Field	Type	Null	Key	Comment
countyID	int(11)	NO	PRI	
monthID	smallint(6)	NO	PRI	
SMOKE_SCC	varchar(10)	NO	PRI	The SMOKE Source Classification Code for the emissions, which is the combination of source type, fuel type, road type, and process. The mapping of MOVES process to SMOKE process can be found in the smoke_moves_mapping table in the new database.
SMOKE_mode	varchar(20)	NO	PRI	The type of output for SMOKE, usually a combination of general process (exhaust, evap, refueling, or permeation) and reactive organic carbon type, either GROC or CROC.
pollutantID	smallint(6)	NO	PRI	
pollutantName	varchar(50)	NO	PRI	
Profile Identifier	varchar(10)	NO	PRI	The specific column name depends on the profile set selected. If non-volatility profiles are selected, the column names are togSpeciationProfileID or pmSpeciationProfileID. If ROC profiles are selected, the column names are GROCCode or CROCCode.
profileContribution	double	YES		The ratio of emissions that are mapped to the given speciation profile.
weightedCROCOMRatio / weightedGROCNMOGRatio	double	YES		The ratio to calculate GROC (for gases) or CROC (for PM) based on MOVES output of non-methane organic gases (NMOG) or total organic matter (TOM), respectively. This is used for novel chemical mechanisms like CRACMM.[iv] This column only exists when the user selects the ROC profile set.

Nonroad

The nonroad scripts output two tables. The first, movesoutput_nhtog, is for the NonHAPTOG pollutant and the second, movesoutput_pm, is for $PM_{2.5}$. Each output table follows the same general schema as described in the following table.

Field	Type	Null	Key	Comment
yearID	smallint(5)	NO	PRI	
monthID	smallint(6)	NO	PRI	
countyID	int(10)	NO	PRI	
pollutantID	smallint(6)	NO	PRI	
pollutantName	varchar(50)	NO	PRI	
processID	smallint(5)	NO	PRI	
fuelSubtypeID	smallint(5)	NO	PRI	
SCC	varchar(10)	NO	PRI	
engTechID	smallint(5)	NO	PRI	
hpID	smallint(5)	NO	PRI	
tierID	smallint(5)	NO	PRI	
strokes	smallint(5)	NO	PRI	Specifies 2- or 4-stroke engine, differentiated for gasoline engines only
emissionQuant	double	YES		MOVES emissions
Profile Identifier	varchar(10)	NO	PRI	The specific column name depends on the profile set selected. If non-volatility profiles are selected, the column names are togSpeciationProfileID or pmSpeciationProfileID. If ROC profiles are selected, the column names are GROCCode or CROCCode.
CROCOMRatio / GROCNMOGRatio	double	YES		The ratio to calculate GROC (for gases) or CROC (for PM) based on MOVES output of non-methane organic gases (NMOG) or total organic matter (TOM), respectively. This is used for novel chemical mechanisms like CRACMM.[iv] This column only exists when the user selects the ROC profile set.

[i] https://www.cmascenter.org/smoke/
[ii] USEPA (2022), SPECIATE5.2 https://www.epa.gov/air-emissions-modeling/speciate
[iii] Murphy B. et al (2023). Reactive Organic Carbon Air Emissions from Mobile Sources in the United States, Atmospheric Chemistry and Physics, *in review*
[iv] https://www.epa.gov/system/files/documents/2021-11/cracmm-factsheet-october-2021-v2.pdf