

Instructions for speciating onroad emissions

Introduction

This document provides instructions for using the post-processing script that calculates speciation profile weights used to speciate onroad residual total organic gases (NONHAPTOG), total organic matter (TOM), and residual particulate matter (nonSO4nonECnonOM) for MOVES version 3.0.4 and later. 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. This script is designed in particular for users interested in running SMOKE and includes 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 hosted on EPA's SPECIATE database.ⁱ For onroad, some gases and PM species are calculated by MOVES 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 report Speciation of Total organic Gas and Particulate Matter in MOVES3 (EPA-420-R-22-017).

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 can also be speciated by post-processing emissions with this script.

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.

The script also provides a ratio that can be used to calculate Condensable and Gaseous Reactive Organic Carbon (CROC and GROC, respectively) to support speciation using the new ROC framework.ⁱⁱ Finally, the script also handles the conversion from MOVES SCC output into SMOKE SCC format.

Instructions

The speciation script can be run from the Tools section of the MOVES GUI, once users have completed the required MOVES runs. For the 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) selected via the Pollutants and Processes panel, along with all prerequisites.

- The MOVES runs must have the following boxes checked in the Output Emissions Detail Panel of the GUI: SCC, source type, fuel type, model year, emission process, regulatory class and road type.
- The MOVES output database containing emissions to be speciated may contain multiple MOVES runs but must only contain output for a single calendar year and single county.

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, saved into the database specified by the user.

Steps to run the Onroad Speciation Profile Weighting 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 Onroad Speciation Profile Weighting Script from the MOVES Tools menu.
3. Select the MOVES output database from Step 1 in the Output Database dropdown menu.
4. 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.
5. Click "Run Profile Weighting Script". Depending on the nature of the run, it may take a couple minutes to complete.

Script Output

The script output writes 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 table follows the same general schema:

Field	Type	Null	Key	Comment
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.
pmSpeciationProfileID / togSpeciationProfileID	varchar(10)	NO	PRI	
pollutantID	smallint(6)	NO	PRI	
pollutantName	varchar(50)	NO	PRI	
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.
countyID	int(11)	NO	PRI	
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. ⁱⁱⁱ

ⁱ USEPA (2022), SPECIATE5.2 <https://www.epa.gov/air-emissions-modeling/speciate>

ⁱⁱ Heald, C. L. and Kroll, J. H. (2020). The fuel of atmospheric chemistry: Toward a complete description of reactive organic carbon, *Science Advances*, 6, eaay8967, DOI:10.1126/sciadv.aay8967

ⁱⁱⁱ <https://www.epa.gov/system/files/documents/2021-11/cracmm-factsheet-october-2021-v2.pdf>