

Instructions for speciating nonroad emissions

Introduction

This document provides instructions for using the post-processing script that provides speciation profiles used to speciate nonroad residual total organic gases (NONHAPTOG) and PM_{2.5} 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 nonroad, some gases are calculated by MOVES directly. These pollutants are referred to as "integrated species." The remaining organic gas emissions are output as NONHAPTOG for post-processing. The list of specific species is detailed in the technical report Speciation Profiles and Toxic Emissions for Nonroad Engines in MOVES3 (EPA-420-R-22-015). Unlike onroad, MOVES has no integrated species for nonroad PM, so post-processing is applied to total PM_{2.5} emissions.

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 script matches MOVES nonroad output to the speciation profile that should be used. 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

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 and PM_{2.5}) 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, fuel type, fuel subtype, and engine tech.
- 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 pair of tables that list the speciation profiles and ratios used for residual TOG and PM, 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 Nonroad Speciation Profile 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 “New 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 Script”. Depending on the nature of the run, it may take a couple minutes to complete.

Script Output

The script output writes two tables. The first, movesoutput_nhtog, is for the NonHAPTOG pollutant and the second, movesoutput_pm, is for PM_{2.5}. Both tables follow the same general schema:

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
pmSpeciationProfileID / togSpeciationProfileID	varchar(10)	NO	PRI	
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. 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>