

BACKGROUND

- Speciation is the process of apportioning organic gas aggregates and particulate matter (PM_{2.5}) emission estimates into specific chemical species for air quality modeling. The apportionment is done using source-specific speciation profiles hosted in EPA's SPECIATE database¹.
- MOVES² provides emissions estimates of TOG and PM_{2.5} for both onroad and nonroad sectors:

ONROAD SPECIATION

For some TOG and PM species, MOVES applies adjustments based on temperature and fuels, that vary by vehicle technology. We refer to these as "integrated species". Subtracting integrated species from TOG provides NONHAPTOG (see Glossary). Subtracting integrated species from total PM_{2.5} provides TOM and Residual PM.

Emissions speciation of onroad NONHAPTOG, TOM and Residual PM has been done in MOVES through selection of chemical mechanisms as a pollutant output.

NONROAD SPECIATION

MOVES does not perform adjustments but provides direct emissions for the same VOCs listed as integrated species and a variety of air toxics including PAHs, dioxins, furans and metals. Nonroad PM_{2.5} is only provided as total PM_{2.5}.

Emissions speciation of nonroad NONHAPTOG and PM_{2.5} has always been done as a post-process.

MOTIVATION

- To allow for timely updates of new chemical mechanisms or speciation profiles with less dependency on MOVES release timing, benefiting the air quality modeling community (e.g., ROC speciation³).
- To facilitate the calculation of chemical mechanisms and reduce model runtime significantly for users that require this output.

PM & TOG Integrated Species

- Methane (CH₄)
- Benzene
- Ethanol
- 1,3-Butadiene
- Formaldehyde
- Acetaldehyde
- Acrolein
- 2,2,4-Trimethylpentane
- Ethyl Benzene
- Hexane
- Propionaldehyde
- Styrene
- Toluene
- Xylene
- Naphthalene gas
- Elemental Carbon
- Sulfate

Glossary

MOVES: MOtor Vehicle Emission Simulator

TOG: Total Organic Gases

NONHAPTOG: Residual TOG (or non-Hazardous Air Pollutant TOG)

TOM: Total Organic Particulate Matter (OM + NCOM)

Residual PM (or NonECNonSO4nonOM): Total PM_{2.5}-EC-SO₄-OC-NCOM

NCOM: Non-carbon Organic Matter

OC: Organic Carbon

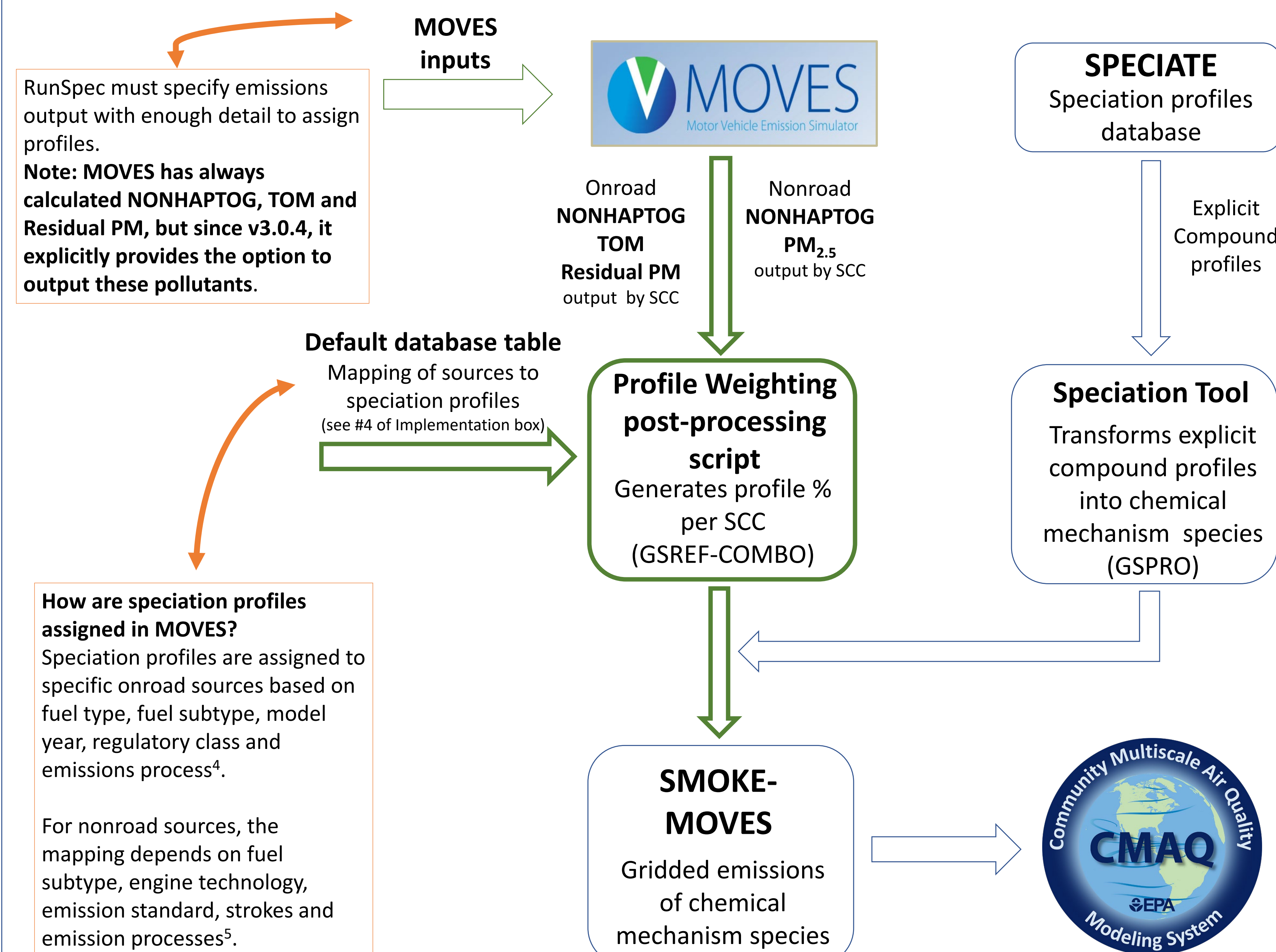
PAH: Polycyclic Aromatic Hydrocarbons

SCC: Source Classification Code

References

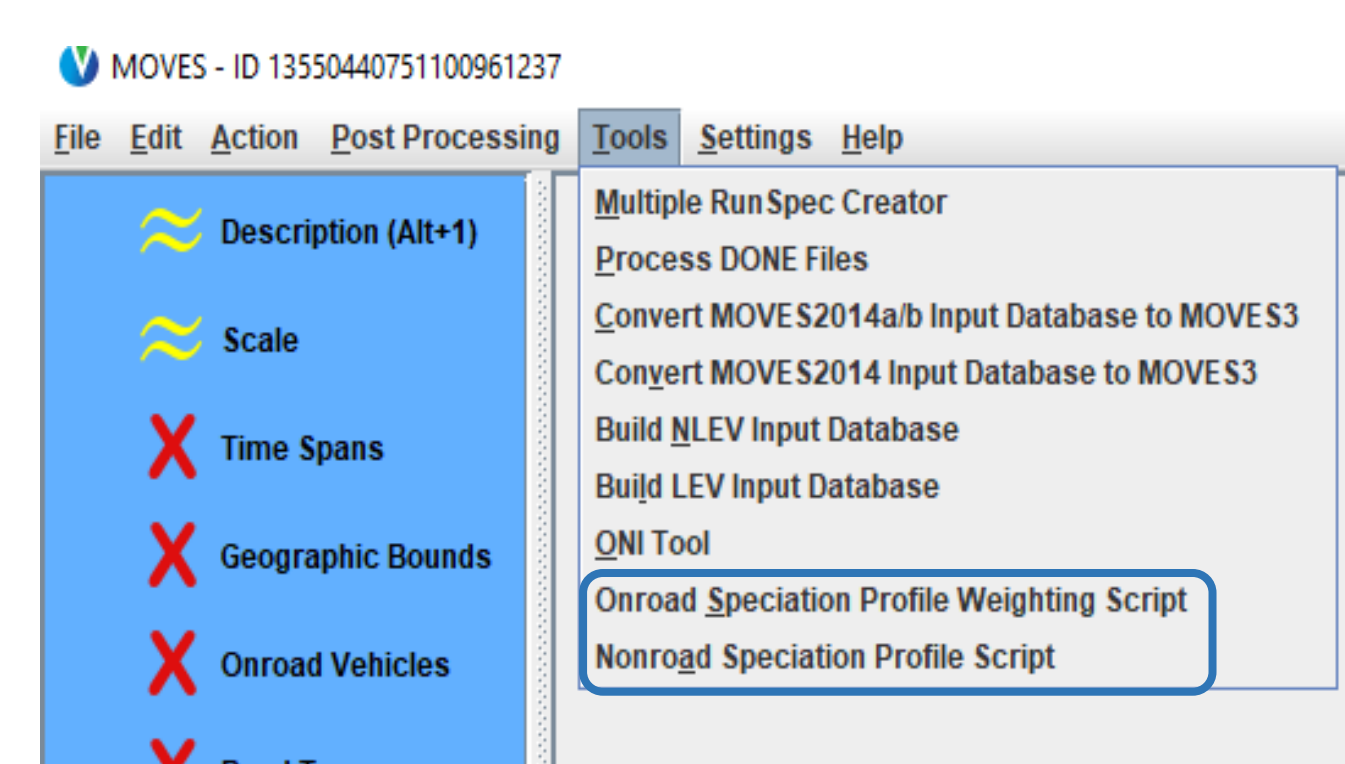
- EPA's SPECIATE database: <https://www.epa.gov/air-emissions-modeling/speciate>
- MOVES, <https://www.epa.gov/moves>
- Murphy et al. (2022), Quantifying the Impact of Mobile-Source Reactive Organic Carbon Emissions on U.S. Air Quality, CMAS Conference Poster
- Speciation onroad, <https://www.epa.gov/moves/moves-onroad-technical-reports>
- Speciation nonroad, <https://www.epa.gov/moves/nonroad-technical-reports>
- CMAQ fact sheets, <https://www.epa.gov/cmaq/cmaq-fact-sheets>

OFFLINE SPECIATION FRAMEWORK



POST-PROCESS IMPLEMENTATION

1. Post-processing script is written in SQL and can be accessed from the MOVES3 GUI



3. Output generates a SQL database with 6 different tables, each associated with an emission process and pollutant type: permeation (EPM), evaporative (EVP), exhaust (EXH) and refueling (RFL) for NONHAPTOG (GROC), TOM (CROC) and ResidualPM.

Table Name
epm_groc
evp_groc
exh_groc
exh_residpm
rfl_groc
smoke_moves_mapping

Example rows from exh_groc output:

month ID	SMOKE_SCC	pmSpeciation ProfileID	pollutant ID	pollutant Name	SMOKE_mode	county ID	profileContribution	weighted CROCOM Ratio
1	2202310192	8995	123	TOM	EXH_CROC	1089	0.98915	0.867
1	2202310192	8996	123	TOM	EXH_CROC	1089	0.01085	2.51642
1	2202310272	8995	123	TOM	EXH_CROC	1089	0.973171	0.867
1	2202310272	8996	123	TOM	EXH_CROC	1089	0.026829	3.33706

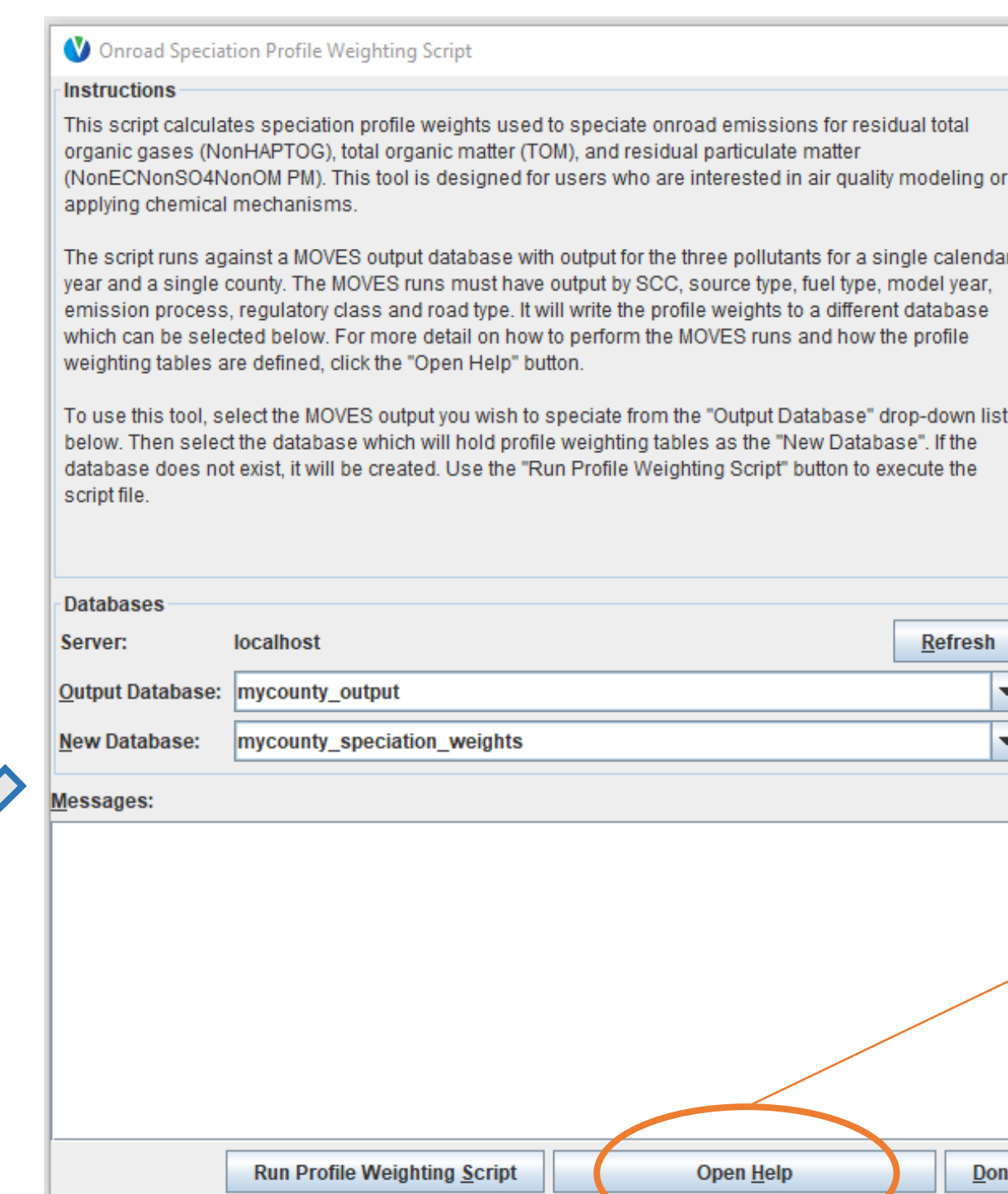
4. Ancillary information

Mapping of sources to speciation profiles is stored in the default database in ancillary tables only used by the post-processing tool

Example rows from rocspeciation table for onroad mapping:

fuelSub	regClass	process	minModel	maxModel	YearID	ProfileID	CROCCode	CROCOM Ratio	logSpeciation ProfileID	GROCCode	GROCCOMOG Ratio
10	20	1	1960	2000	8993	101CROC	1.369	8751a	102GROC	1	1
10	20	15	1960	2000	8993	101CROC	1.369	8751a	102GROC	1	1
11	20	1	1960	2000	8993	101CROC	1.369	8751a	102GROC	1	1
11	20	15	1960	2000	8993	101CROC	1.369	8751a	102GROC	1	1
12	20	1	1960	2000	8993	101CROC	1.369	8751a	102GROC	1	1

2. Selecting the tool will open a window containing a description, and a scroll down menus to select input and output databases:



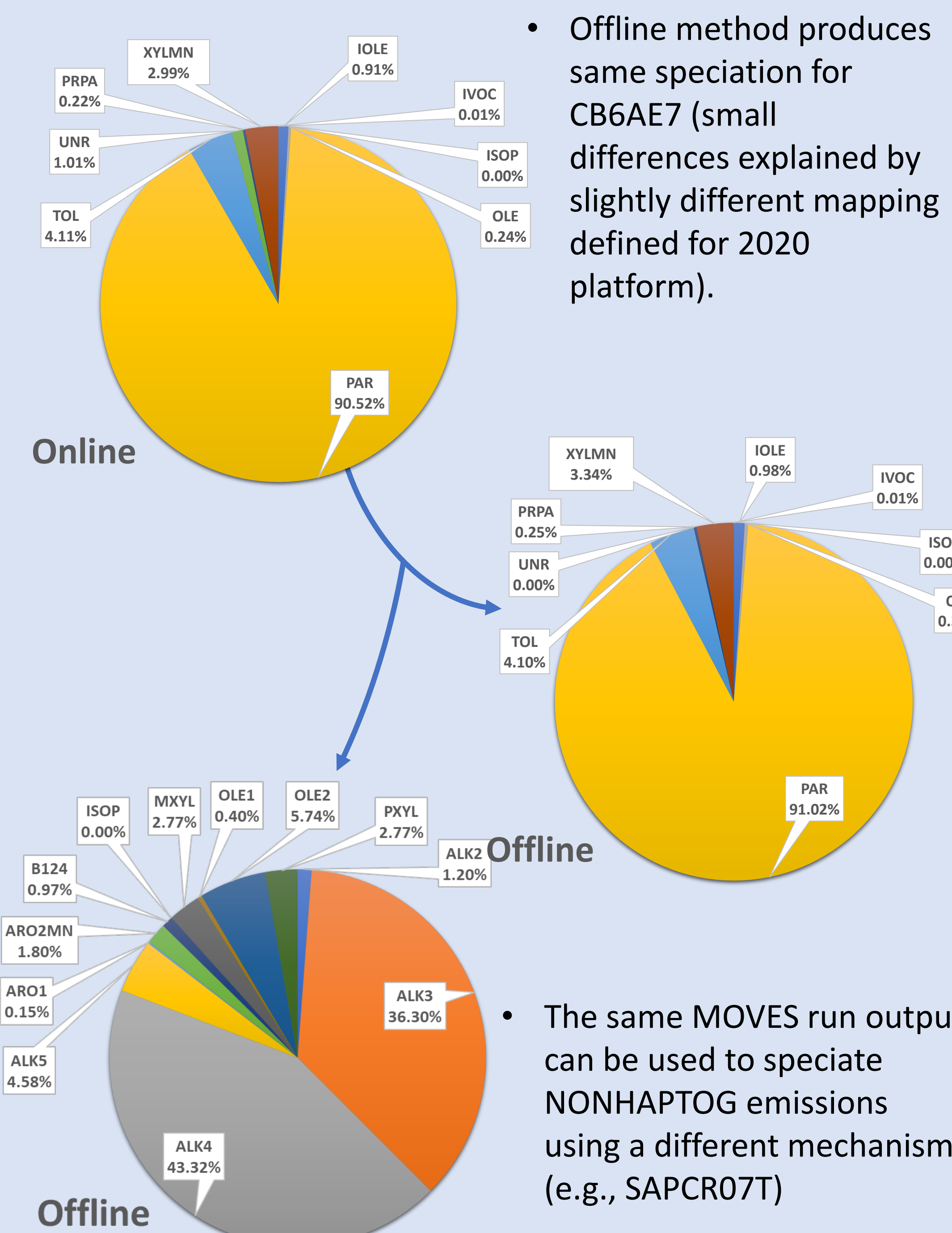
More information if needed!

Profile Contribution parameter represents the fractional contribution of each speciation profile to emissions from a given SCC; it sums up to 1 for each SCC and month.

Parameters shaded in green are used to calculate condensable/gaseous reactive organic carbon emissions for users interested in applying chemical mechanisms that account for them (e.g., CRACMM⁶).
See application in poster by Murphy et al.³

EXAMPLE

- Speciation of evaporative emissions from passenger cars for an example county on a July weekday in 2022 using CB6AE7 via internal speciation (i.e., selecting CB6AE7 as an output pollutant in MOVES3.0.3) and new offline methodology in MOVES3.0.4:



- Offline method produces same speciation for CB6AE7 (small differences explained by slightly different mapping defined for 2020 platform).

- The same MOVES run output can be used to speciate NONHAPTOG emissions using a different mechanism (e.g., SAPCRO7T)

HIGHLIGHTS

- MOVES3 (v3.0.4 and after) no longer provides output speciated into model species (chemical mechanisms).
- Users that need to speciate onroad and/or nonroad gaseous or PM emissions should use a post-processing script included in the Tools menu of the MOVES3 GUI.
- The post-processing provides weights representing the fraction of emissions that should be assigned to a specific SPECIATE profile for a given SCC. These profile weights are used downstream in SMOKE.
- Moving the speciation process outside of MOVES allows using SMOKE capabilities to handle speciation profiles defined under different mechanisms without performing new MOVES runs.
- Providing an external tool facilitates the incorporation of new data and science related to speciation profiles or chemical mechanisms for onroad and nonroad sources as it becomes available (e.g., ROC speciation³).