Speciation of Total Organic Gas and Particulate Matter Emissions from Onroad Vehicles in MOVES201X

July, 2017

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U.S. Environmental Protection Agency

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1 Introduction

In addition to estimating emissions of pollutants that are discrete chemical compounds, such as carbon monoxide (CO) and sulfur dioxide (SO_2), MOVES produces emission rates for aggregates of individual chemical compounds, including total hydrocarbons (THC), volatile organic compounds (VOC), total organic gases (TOG) and particulate matter (PM). These pollutants are operationally defined, meaning that their definition depends on the measurement technique(s) selected. For example, THC is defined as the hydrocarbons measured by a flame ionization detector (FID). TOG is defined to include all organic gases.[1] Because THC measurements do not respond fully to carbon-oxygen bonds in oxygenated compounds, such as aldehydes, alcohols, and ketones, these oxygenates need to be measured separately by gas and liquid chromatography and added to the THC measurements to calculate TOG. Alternatively, TOG measurements can be made solely with gas and liquid chromatography methods.[a] Similarly, particulate matter is operationally defined as the measured mass collected on a filter using EPA-defined sampling filter media, conditions, and practices.[2,3] $PM_{2.5}$ refers to particulate matter emissions collected downstream of a cyclone that removes the particles with aerodynamic diameter greater than 2.5 microns, while PM_{10} refers to particulate matter emissions with aerodynamic diameter less than 10 microns.

MOVES produces emission estimates for a subset of species that contribute to TOG and $PM_{2.5}$. These include important organic gaseous toxics (e.g., formaldehyde and benzene), and toxic particle-phase elements (e.g., nickel and manganese). These also include semi-volatile organic compounds, such as 15 individual polycyclic aromatic hydrocarbons (e.g., benzo(*g*,*hi*,*i*)perylene) that can exist in both the gaseous and particle phases under different measurement conditions. Individual toxic emission rates are detailed in the toxics report[4], but are peripherally discussed in this report in the context of their use in deriving speciated TOG and PM emissions.

For air quality modeling purposes, further chemical characterization of TOG and $PM_{2.5}$ is required. The process of apportioning aggregate TOG and $PM_{2.5}$ into sets of separate components is called "speciation." MOVES incorporates the process of TOG and $PM_{2.5}$ speciation to produce the TOG and $PM_{2.5}$ species needed by air quality models. This improves accuracy and flexibility since TOG and $PM_{2.5}$ speciation depends on technology, fuels and emission processes. By incorporating the speciation process, MOVES can readily calculate the speciated components of TOG and $PM_{2.5}$ on a model year, fuel, vehicle class and emission-process basis in order to reflect distinctions in different TOG and $PM_{2.5}$ profiles.

This document is intended to comprehensively describe all the data and calculations used by MOVES201X in speciation calculations, including those that are unchanged from previous versions of MOVES. In addition, we have also highlighted the updates made in MOVES201X, specifically regarding the calculation of TOG species. In MOVES, the determination of organic compounds is done through a chain of calculations involving ratios of organic aggregates such as methane-to-THC ratios (CH_4/THC), NMOG-to-NMHC ratios (NMOG/NMHC) and VOC-to-NMHC ratios (VOC/NMHC). In previous versions of MOVES, these ratios were calculated

[a] Thus, differences in measurement methods need to be considered when comparing THC to TOG emission measurements.

based on available data and on empirical constants derived to correct for adjustments related to the oxygen content in fuels.

However, in MOVES201X, we calculate the CH_4/THC ratios based on profiles from the SPECIATE database. In addition, we calculate NMOG/NMHC and VOC/NMHC for each of the SPECIATE profiles, ensuring consistency throughout the TOG calculation chain. Besides simplifying TOG calculations, this methodology more directly relates organic compound emissions to multiple combinations of MOVES classifications (model year groupings, regulatory class, fuel subtype and emissions process). Furthermore, it provides flexibility to incorporate new data into MOVES as they become available. In the case of Tier 2 vehicles using low-level ethanol blends, we updated CH_4/THC, NMOG/NMHC and VOC/NMHC ratios using bag-specific data from the EPAct Phase 1 program[5] whereas data from the EPAct/V2/E89 program[6] was used for vehicles running on E85.

A consequence of the changes made in MOVES201X is that empirical constants used to correct for oxygen content in fuels (oxySpeciation, volToWtPercentOxy, oxyVolume) in previous versions cannot be estimated with this new methodology. MOVES has fuel subtypes for different compositions of ethanol (E0, E5, E8, E10, E15, E20, E85), accounting for the main oxygenated fuels distributed, but the new methodology removes the capability of MOVES to adjust NMOG and VOC according to other oxygenated compounds such as methyl tert-butyl ether (MTBE), ethyl tert-butyl ether (ETBE) and tert-amyl methyl ether (TAME). These other oxygenated compounds are no longer used in the US fuel supply, and are not expected to return, which supports the removal of modeling capabilities for fuels containing these types of additives.

This report has been revised for MOVES201X from the previous version (EPA-420-R-15-022).[7] These changes include: updates to total organic gases calculations (Section 3), updates to the calculation of chemical mechanisms species (Section 4) and incorporation of a new $PM_{2.5}$ exhaust profile for 2010 and later heavy-duty diesel vehicles (Section 5).

2 Speciation Glossary

In the area of "speciation," many terms have two or more meanings. The list below defines them to avoid confusion. The current report tries to use unambiguous terms that are close to the common usage.

- Aggregate species: Groups of chemical compounds (or “real species”). These are often defined operationally or may be defined for modeling purposes. For example, THC, TOG and VOC are aggregate gaseous species. NonEC is an aggregate particulate matter species.

- Elemental Carbon (EC): “A descriptive term for carbonaceous particles based on chemical composition rather than light-absorbing characteristics. This term is often used as a synonym for black carbon.”[8] Elemental carbon is measured through thermal optical techniques as particle-phase carbon that does not volatize at high temperatures in an oxygen-free environment.[9] In tailpipe exhaust, EC is one measure of carbonaceous soot formed from fuel pyrolysis occurring during combustion.[10]

- CMAQ: The Community Multiscale Air Quality system is a photochemical and transport air quality model. CMAQ is an open source development project sponsored by the US EPA Atmospheric Science Modeling Division (https://www.cmascenter.org/cmaq/).

- Chemical mechanism: In air-quality models, chemical mechanisms are simplified representations of the full panoply of atmospheric chemical reactions. They have been developed by air-quality modelers to speed up the atmospheric chemistry calculations in their models. An aspect of these chemical mechanisms is the use of a relatively small set of "chemical mechanism species," (CM species) into which all the real species can be mapped, and which serve to model the atmospheric reactions of importance. For the purposes of MOVES, a chemical mechanism may be thought of as a set of CM species and the mapping between regular MOVES output species and the CM species. MOVES201X can produce inventory and rates output for CM species for three chemical mechanisms: CB05,[11] CB6CMAQ,[12] and SAPRC07T.[13] Furthermore, since the mapping is table-driven, MOVES has the structure in place to generate CM species for any chemical mechanism.

- Integrated species: Real species for which MOVES produces emissions that are subtracted from TOG, leaving residual TOG. This residual TOG is speciated into CM species using a CM speciation profile constructed from the real speciation profile from which the integrated species have been removed. The integrated species, which are produced by MOVES, are individually speciated into CM species. At present, MOVES integrates the 16 species shown in Table 2-1. MOVES is designed to accept different sets of integrated species, if desired.

Table 2-1 Integrated MOVES Pollutants

pollutantID	Pollutant Name
5	Methane (CH_4)
20	Benzene
21	Ethanol
22	MTBE
24	1,3-Butadiene
25	Formaldehyde
26	Acetaldehyde
27	Acrolein
40	2,2,4-Trimethylpentane
41	Ethyl Benzene
42	Hexane
43	Propionaldehyde
44	Styrene
45	Toluene
46	Xylene
185	Naphthalene gas

- Intermediate $PM_{2.5}$ species: Groups of $PM_{2.5}$ species used to improve computation time, and reduce the size of the emission rate tables. They include the aggregate species: "non-elemental carbon particulate matter" (NonECPM) and "non-elemental carbon non-sulfate particulate matter" (NonECnonSO_4PM), elemental carbon (EC), sulfate (SO_4) and particulate water (H_2O). They are used to compute total $PM_{2.5}$ emissions and speciated $PM_{2.5}$ emissions. The EC, SO_4, and H_2O species are reported as MOVES outputs.

- Chemical Mechanism species (CM species): the species used by chemical mechanisms. CM species include both artificial constructs (sometimes referred to as "lumped species") and real species. CM species are unique to particular chemical mechanisms (e.g., CB05, SAPRC07). All real TOG species are mapped to CM species. For a particular chemical mechanism, the associated group of CM species can be referred to by the name of the mechanism, for example, CB05 species.

- CM speciation profile: the mapping of a real species (e.g., hexane) or an aggregate species (e.g., TOG) into CM species. The mapping of real species into CM species has been created by the developers of chemical mechanisms for air quality modeling[11,12,13].

- The mapping of real species is independent of process and fuel. The mapping of aggregate species (e.g., residual TOG) represents the sum of the mappings of the individual real species from the real speciation profiles. The mapping of aggregate species depends on process and fuel.

- Organic Mass (OM): Particle-phase organic mass. The mass of the organic material in particulate: OM = organic carbon (OC) + non-carbon organic matter (NCOM).

- Organic Carbon (OC): "The mix of compounds containing carbon bound with other elements; e.g., hydrogen and oxygen. Organic carbon may be a product of incomplete combustion, or formed through the oxidation of VOCs in the atmosphere." Organic carbon is measured using thermal-optical methods as the particle-phase carbon collected on a filter that volatizes at high temperatures in an oxygen-free environment.

- Non-Carbon Organic Mass (NCOM): the mass of the oxygen, hydrogen, nitrogen and other elements present in particle-phase organic mass. OC and NCOM are modeled separately in air quality models in order to model the degree of oxidation of organic matter, which depends on the emission source and the chemical transformation in the atmosphere.[14]

- Non-Elemental Carbon Particulate Matter (nonECPM): The $PM_{2.5}$ that is not elemental carbon. This is typically calculated as the difference between $PM_{2.5}$ mass filter-based measurements and elemental carbon measurements made using thermal optical measurements, or surrogate elemental carbon measurements such as photoacoustic sensors. $nonECPM = nonECnonSO_4PM + SO_4 + H_2O$.

- Non-Elemental Carbon, Non-Sulfate Particulate Matter (nonECnonSO_4PM): MOVES intermediate species used to represent the $PM_{2.5}$ mass other than elemental carbon, sulfate, and associated water. NonECnonSO_4PM includes organic matter, elements, and ions. NonECnonSO_4PM is adjusted for fuel and temperature effects prior to speciation due to limited data on temperature and fuel effects on individual $PM_{2.5}$ species in the exhaust, and to improve computational time.

- Non-Methane Hydrocarbons (NMHC): NMHC = THC – CH_4 (methane).

- Non-Methane Organic Gases (NMOG): NMOG = TOG – CH_4 (methane).

- Real species: "Species" in the normal chemical sense—a pure chemical substance. The word "real" helps distinguish these species from chemical mechanism species or aggregated species.

- Real speciation profile: ideally, a complete listing of the real species and their quantities of TOG. In practice, these profiles are incomplete; a certain fraction of the mass is unresolved. Such a profile is produced by laboratory analysis of emissions. This is not a CM speciation profile and is independent of chemical mechanism. Such a profile does, however, depend on process, fuel, and technology, since the mix of real species in TOG is different for different emission processes (e.g. evaporative and exhaust), for different fuels, and for different technologies. The SPECIATE database is the EPA repository for these profiles. (https://www.epa.gov/air-emissions-modeling/speciate-version-45-through-40)

- Residual TOG: TOG that remains after subtracting integrated species.

- Primary Exhaust $PM_{2.5}$ - Total ($PM_{2.5}$). Primary particulate matter emissions from vehicle exhaust collected filter, measured downstream of a cyclone that removes the particles with aerodynamic diameter greater than 2.5 microns. $PM_{2.5}$ = EC + nonECPM.

- Process: MOVES has twelve emission processes that are relevant for TOG speciation. The processID and names are included in Table 2-2. Within each process, emission rates can potentially vary by operating mode. Running exhaust has different operating modes to represent idling, coasting, and operating with different engine loads. Start exhaust has different operating modes to differentiate a continuum of starts between cold, warm, and hot starts. The operating modes are defined in the MOVES201X emission rate report[41], and the evaporative report.[15] In MOVES, different TOG and PM speciation profiles can be applied to different processes, but not to individual operating modes.

Table 2-2 MOVES Processes Relevant for Speciation Profiles

processID	Process Name
1	Running Exhaust
2	Start Exhaust
11	Evap Permeation
12	Evap Fuel Vapor Venting
13	Evap Fuel Leaks
15	Crankcase Running Exhaust
16	Crankcase Start Exhaust
17	Crankcase Extended Idle Exhaust
18	Refueling Displacement Vapor Loss
19	Refueling Spillage Loss
90	Extended Idle Exhaust
91	Auxiliary Power Exhaust

- Source Classification Code (SCC): Standard code that identifies various emissions sources for inventory reporting and air quality modeling.

- SMOKE: Sparse Matrix Operator Kernel Emissions is a computer program used to provide model-ready inputs into CMAQ. SMOKE produces gridded, speciated, and hourly emissions input for use in CMAQ and other air-quality models. (https://www.cmascenter.org/smoke/)

- Species: Distinct chemical compounds, ions, groups of compounds, or other chemical entities. In this report, we distinguish “real species,” “aggregate species,” “CM species,” and “intermediate species,” as explained above.

- Total Hydrocarbons (THC): “THC is the measured hydrocarbon emissions using a Flame Ionization Detector (FID) calibrated with propane. The FID is assumed to respond to all hydrocarbons identically as it responds to propane in determining the concentration of carbon atoms in a gas sample. Most hydrocarbons respond nearly identically as propane with notable exceptions being oxygenated hydrocarbons such as alcohols and aldehydes commonly found in engine exhaust.” [1]

- Total Organic Gases (TOG): hydrocarbon emissions plus oxygenated hydrocarbons such as alcohols and aldehydes.[1]

- Volatile Organic Compounds (VOC): TOG emissions minus those hydrocarbons that contribute little to ozone formation, such as methane, ethane, and acetone.[1] EPA may over time exclude additional organic compounds from the definition of VOC which have negligible photochemical reactivity. For the current list, see: Code of Federal Regulations, 40: Chapter 1, Subchapter C, Part 51, Subpart F, 51100(s). In mobile source testing, typically only a few compounds with negligible photochemical reactivity are measured in significant quantities. For the TOG speciation profiles used in MOVES, VOC is defined as TOG minus methane, ethane, and acetone.

3 Organic Gas Aggregations

MOVES provides estimates of organic gas emissions in a number of different aggregations. Table 3-1 shows the composition of various organic gas aggregate classes in MOVES. As the table shows, the organic gas aggregations differ based on the presence or absence of methane, ethane, alcohols, and aldehydes. Definitions of these species are also included in the glossary. The term "FID-HC" refers to the total hydrocarbons detected by a Flame Ionization Detector (FID). In MOVES, THC (pollutantID=1) is defined as FID-HC, and thus, includes methane and ethane. MOVES calculates emissions of total organic gases (TOG), non-methane organic gases (NMOG) and volatile organic compounds (VOC) using information regarding the total organic gas speciation of emissions.

Table 3-1. Relationships among Organic Gas Aggregations in MOVES

pollutantID	pollutantName	FID-HC	Methane	Ethane	Acetone	Alcohols	Aldehydes
1	Total Hydrocarbons	Yes	Yes	Yes	No	No	No
79	Non-Methane Hydrocarbons	Yes	No	Yes	No	No	No
87	Volatile Organic Compounds	Yes	No	No	No	Yes	Yes
86	Total Organic Gases	Yes	Yes	Yes	Yes	Yes	Yes
80	Non-Methane Organic Gases	Yes	No	Yes	Yes	Yes	Yes

In MOVES, THC emission rates are the base emission rates (field meanBaseRate in the EmissionRateByAge table) from which each of the other organic emissions are estimated. The following section presents the equations used to derive these other aggregate organic gas emission rates from THC.

3.1.Total Organic Gaseous Calculations

Exhaust regulations for organics are often expressed in terms of non-methane hydrocarbons (NMHC). MOVES calculates both methane and NMHC from the THC emissions using methane-to-total hydrocarbon ratios (field CH4THCRatio in the MethaneTHCRatio table) as shown in Equation 1 and Equation 2.

$$CH_4 = THC \times \frac{CH_4}{THC}$$ **Equation 1**

$$NMHC = THC \times \left(1 - \frac{CH_4}{THC}\right)$$ **Equation 2**

Following the calculation of NMHC, the MOVES algorithm calculates NMOG, VOC and TOG as shown in Equation 3 through Equation 5.

$$NMOG = NMHC \times \frac{NMOG}{NMHC}$$ **Equation 3**

$$VOC = NMHC \times \frac{VOC}{NMHC} \quad \textbf{Equation 4}$$

$$TOG = NMOG + CH_4 \quad \textbf{Equation 5}$$

In previous versions of MOVES, the data used to calculate CH_4/THC was not consistent with the data used to calculate ratios of organic aggregates that followed in the calculation chain within MOVES.[16] Therefore, for MOVES201X, we determine CH_4/THC from SPECIATE profiles that are currently used in the model. The methodology to calculate ratios from SPECIATE data is presented in Section 3.1.1 and the calculated ratios for each profile are presented in Table 3-2.

The NMOG/NMHC and VOC/NMHC ratios shown in Equation 3 and Equation 4 are referred within MOVES as speciationConstant and stored in the HCSpeciation table. In MOVES201X, speciationConstant parameters were calculated for each SPECIATE profile currently used in MOVES in order to be consistent with the updated CH_4/THC ratios included in this release and with the TOG calculation chain.[b] These ratios continue to be stored in the HCSpeciation table which now also includes the fields regClassID and fuelSubtypeID. The new speciationConstant parameters are also presented in Table 3-2.

The calculation of NMOG and VOC in previous MOVES versions included additional terms that represented adjustments to correct for the oxygenated volume in the fuel (oxySpeciation, volToWtPercentOxy and oxyVolume parameters). In this latest release, the adjustments made to correct for oxygenated volume in the fuel were removed, simplifying the equations as shown in Equation 3 and Equation 4. The fuel market projections indicate that additives other than ethanol are unlikely to return to the market, supporting the removal of these parameters from the model.

[b] Previous to MOVES201X, the speciationConstant parameters were calculated using either of two methods. The first method was based on the relative carbon fraction of each species and was first developed for MOBILE4.1. The second method was based on Equation 1066.635-1 of the CFR. For further details, the reader is directed to the Speciation of Total Organic Gas and Particulate Matter Emissions from On-road Vehicles in MOVES2014 report (EPA-420-R-14-022).

Table 3-2 Updated CH_4/THC and speciationConstant Parameters from SPECIATE Profiles for MOVES201X

Profile Number	Profile Description	Emission Process	Fuel Subtype	Affected Vehicles	CH_4/THC Ratio	NMOG/NMHC Ratio	VOC/NMHC Ratio
4547	Diesel headspace	Evaporative Permeation	Diesel, biodiesel	All diesel	0	1	1
8750a	Pre-Tier 2 E0 exhaust	Running, starts exhaust and crankcase	Conventional Gasoline	Pre-2001 LD gasoline	0.142	1.024	0.996
				All MC and non-LD gasoline			
8751a	Pre-Tier 2 E10 exhaust	Running, starts exhaust and crankcase	RFG, E10, E8, E5	Pre-2001 LD gasoline	0.146	1.037	1.008
				All MC and non-LD gasoline			
8753	E0 Evap	Evaporative (vapors, leaks), refueling spillage	Conventional Gasoline	All gasoline	0	1	1
8754	E10 Evap	Evaporative (vapors, leaks), refueling spillage	E10, E8, E5	All gasoline	0	1.071	1.071
8766	E0 Evap perm	Evaporative Permeation	Conventional Gasoline	All gasoline	0	1	1
8769	E10 Evap perm	Evaporative Permeation	E10, E8, E5	All gasoline	0	1.129	1.129
8770	E15 Evap perm	Evaporative Permeation	E15, E20	All gasoline	0	1.175	1.175
8774	Pre-2007 MY HDD exhaust	Running, starts, extended idle exhaust and crankcase	Diesel, biodiesel	Pre-2007 diesel	0	1.145	1.124
		APU		Pre-2024 APU			
		Running, starts exhaust and crankcase		Pre-2007 LD diesel			
8775	2007-2009 HDD exhaust	Running, starts exhaust and crankcase	Diesel, biodiesel	2007+ LD diesel	0.589	1.343	1.285
		APU		2024+ APU			
		Running, starts, extended idle exhaust and crankcase		2007+ HD diesel			
9335	2010+ HDD exhaust	Running, starts exhaust and crankcase	Diesel, biodiesel	2010+ LD diesel	0	1.085	0.965
		Running, starts, extended idle exhaust and crankcase		2010+ HD diesel			

Table 3-2 (continued)

<table>
<tr><th>Profile Number</th><th>Profile Description</th><th>Emission Process</th><th>Fuel Subtype</th><th>Affected vehicles</th><th>CH_4/THC Ratio</th><th>NMOG/NMHC Ratio</th><th>VOC/NMHC Ratio</th></tr>
<tr><td>8869</td><td>E0 Headspace</td><td>Refueling displacement vapor loss</td><td>Conventional gasoline</td><td>All gasoline</td><td>0</td><td>1</td><td>1</td></tr>
<tr><td>8870</td><td>E10 Headspace</td><td>Refueling displacement vapor loss</td><td>E10, E8, E5</td><td>All gasoline</td><td>0</td><td>1</td><td>1</td></tr>
<tr><td>8871</td><td>E15 Headspace</td><td>Refueling displacement vapor loss</td><td>E15, E20</td><td>All gasoline</td><td>0</td><td>1</td><td>1</td></tr>
<tr><td>8872</td><td>E15 Evap</td><td>Evaporative (vapors, leaks), refueling spillage</td><td>E15, E20</td><td>All gasoline</td><td>0</td><td>1.118</td><td>1.118</td></tr>
<tr><td rowspan="2">8934</td><td rowspan="2">E85 Evap</td><td>Evaporative permeation</td><td rowspan="2">E85, E70</td><td>All gasoline vehicles running on high ethanol blends</td><td rowspan="2">0</td><td rowspan="2">1.501</td><td rowspan="2">1.501</td></tr>
<tr><td>Evaporative (vapors, leaks), refueling displacement and spillage losses</td><td>All gasoline vehicles running on high ethanol blends</td></tr>
</table>

3.1.1. CH_4/THC and speciationConstant Parameters Using SPECIATE Profiles

We use SPECIATE profiles to derive the speciation constants for all emissions processes/vehicle classes except exhaust from 2001 and later light-duty vehicles; for these, we use bag-specific data from the EPAct/V2/E-89 program to derive the exhaust speciation constants, as discussed in Section 3.1.2.

The speciation profiles in MOVES were obtained from the SPECIATE database version 4.5. Each profile has a detailed list of measured compounds and reports their weight as percentage of TOG. The calculation of NMOG for each profile was done by simply subtracting CH_4 from TOG as shown in Equation 6.

$$NMOG = TOG - CH4 \qquad \textbf{Equation 6}$$

The calculation of NMHC is based on Equation 1066.635-1 in the Code of Federal Regulations. The equation provided in the CFR was rearranged as shown in Equation 7 to solve for NMHC using NMOG calculated in the previous step as an input.

$$m_{NMHC} = m_{NMOG} + \rho_{NMHC} \times \sum_{i=1}^{N} \frac{m_{OHCi}}{\rho_{OHCi}} \times RF_{OHCi_{[THC-FID]}} - \sum_{i=1}^{N} m_{OCHi} \qquad \textbf{Equation 7}$$

Where:

m_{NMOG} = mass of NMOG in the exhaust.
m_{NHMC} = mass of NMHC in the exhaust.
ρ_{NMHC} = 576.816 g/m3 which is the effective C1-equivalent density of NMHC as specified in §1066.1005(f).
m_{OHCi} = mass of oxygenated species i in the exhaust.
ρ_{OHCi} = C1-equivalent density of oxygenated species i as specified in 40 CFR 1066.605-1. For methanol, the density is 1332.02 g/m^3; for ethanol, the density is 957.559 g/m^3; for acetaldehyde, the density is 915.658 g/m^3; for formaldehyde, the density is 1248.21 g/m^3; and for propanol, the density is 832.74 g/m^3.
$RF_{OHCi[THC\text{-}FID]}$ = response factor of a THC-FID to oxygenated species i relative to propane on a C1-equivalent basis as determined in 40 CFR 1065.845. The RF for acetaldehyde is 0.5; for formaldehyde is 0; for ethanol is 0.75; for methanol is 0.63 and for propanol is 0.85.

After NMHC and NMOG are calculated, the calculation of THC is done as shown in Equation 8. Once THC is calculated, the CH_4/THC can then be determined.

$$THC = NMOG \times \frac{NMHC}{NMOG} + CH_4 \qquad \textbf{Equation 8}$$

Finally, VOC is calculated following the definition used in MOVES, where hydrocarbons with a small contribution to ozone formation[17] (specifically methane, ethane and acetone) are subtracted from the TOG as shown in Equation 9.

$$VOC = TOG - CH_4 - C_2H_2 - C_3H_6O \qquad \textbf{Equation 9}$$

Table 3-2 presents all the ratios determined for each SPECIATE composite profile. Information on the data behind each SPECIATE profile is provided in more detail in Table A-4.

Table 3-2 notes the assignment of the derived speciation ratios to different model years, processes, fuel subtypes, and regulatory classes. For gasoline exhaust, we use profiles 8750a and 8751a to represent gasoline exhaust for 2000 and earlier light-duty vehicles. For other gasoline regulatory classes (motorcycles and heavy-duty vehicles), the same profiles were used for all model years.

For vapor venting, fuel leaks, and fuel spillage loss emissions from E0, E10, and E15 fuels, the speciation constants are based on SPECIATE profiles from the Auto/Oil Air Quality Improvement Research Program. Separate speciation constants for gasoline refueling displacement vapor loss were derived for these same fuels using different SPECIATE profiles from the same program. The speciation constants for all refueling and vapor loss emission processes for E15 fuels are based on SPECIATE profiles from a composite profile developed from data collected in the Auto/Oil Air Quality Improvement Research Program and EPAct/V2/E-89 program. For evaporative permeation emissions (processID 11), MOVES uses speciation constants developed from three ethanol blend levels (E0, E10, E15) from the CRC E-77 program.[18] The speciation constants for all evaporative emission processes from E85-fueled vehicles are calculated from a SPECIATE profile based on a profile developed from the CRC E-80 report.[19] Diesel refueling emissions (which currently only include spillage loss) assumes speciation constants developed from a diesel headspace SPECIATE profile, which has equivalent emissions of THC, NMHC, VOC, and TOG, since no methane, ethane, acetone, formaldehyde, acetaldehyde, or ethanol were measured.

For pre-2007 diesel emissions, MOVES uses speciation profile 8774, which is based on a review of speciated diesel emissions on pre-2007 model year engine technologies. MOVES uses the pre-2007 NMOG/NMHC value for diesel auxiliary power units (APUs; processID 91) for all model years prior to 2024 because they are not subject to the same control as on-highway diesel engines. For 2007 to 2009 main diesel engines, MOVES uses speciation profile (8775) based on data from Phase 1 of the Advanced Collaborative Emissions Study (ACES)[20], which includes diesel engines equipped with particulate filter equipped diesel engines, and is the technology used to meet the heavy-duty 2007 diesel standards.[21] MOVES also applies the ACES Phase 1 speciation profile to 2024 and later auxiliary power units because it is anticipated they would use diesel particulate filters to meet the APU PM standards promulgated as part of the Phase 2 medium and heavy-duty greenhouse gas regulation.[22] For 2010 and later diesel engines, MOVES applies a speciation profile from Phase 2 of the Advanced Collaborative Emissions Study (ACES)[23] which includes 2011 model year engines equipped with diesel particulate filters and selective catalytic reduction systems that are representative of current and future technology diesel engines. The use of ACES Phase 2 profile for characterizing emissions from 2010+ heavy-duty trucks was also recommended by the peer-reviewers of MOVES2014 Speciation report.[7]

3.1.2. CH_4/THC and speciationConstant Parameters not Based on SPECIATE Profiles

3.1.2.1 Tier 2 Vehicles

The determination of CH_4/THC, NMOG/NMHC and VOC/NMHC ratios for Tier 2 vehicles running on ethanol blends was done using bag-specific data from the EPAct Phase 1 program (0 percent -15 percent ethanol) and EPAct/V2/E-89 program (85 percent ethanol).

EPAct Phase 1 was designed to collect data from light-duty vehicles running on low-level ethanol blends. Three vehicles (MY2008) were tested to generate data for the three bags required to create speciated composite profiles. The tests involved 9 runs using fuel with 0 percent ethanol, 6 runs using fuel with 10 percent ethanol and 7 runs using fuel with 15 percent ethanol. Further information on vehicles, fuels and testing is detailed on the EPAct Phase I report.[5] The data corresponding to the runs used for this analysis is listed in Table A-1 in the Appendix.

For ethanol levels between 0-15 percent, the average CH_4 and THC emissions were calculated and subsequently a ratio of means was determined (i.e., CH_4avg/THCavg). To verify if there was a statistically significant trend with ethanol composition, a linear regression between the previously determined ratios and ethanol composition was performed (Figure 3-1). The regression analysis indicated that the slope was statistically significant (significance level < 0.05) for start emissions but not for running emissions. Therefore, CH_4/THC for starts are specific for each ethanol composition, but for running an average CH_4/THC across all low-level ethanol blends is used. The linear fit for starts was used to interpolate CH_4/THC values for E5 and E8 fuel compositions used in MOVES201X for which no SPECIATE profiles are available.

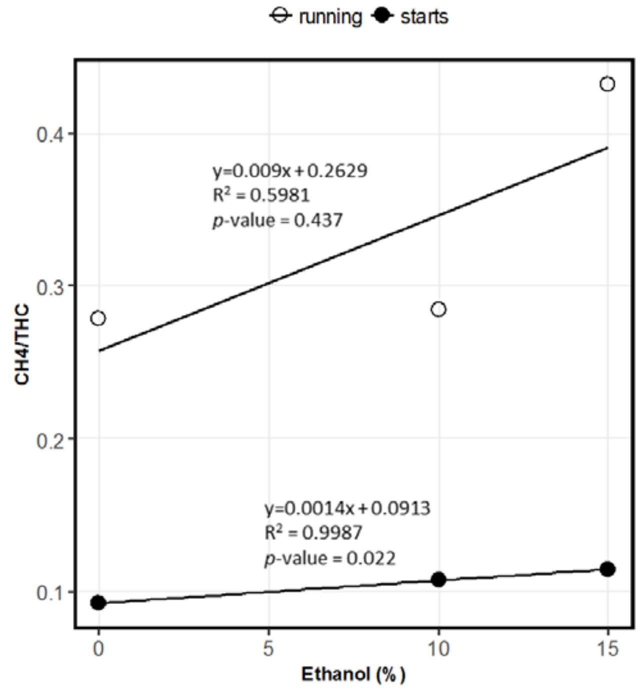

Figure 3-1 Relationship between CH_4/THC Ratios and Ethanol Composition for Tier 2 Vehicles using Low-Level Ethanol Blends

The speciated data used to determine NMOG/NMHC and VOC/NMHC for Tier 2 vehicles corresponds to the same EPAct Phase 1 runs referred to in the determination of CH4/THC ratios for these vehicles. Data from Bag 3 was subtracted from Bag 1 to determine cold start emissions. NMOG, VOC and NMHC were calculated for each test following the methodology described in Section 3.1.2. The reported speciationConstant parameters were determined as a ratio of means (i.e., NMOGavg/NMHCavg or VOCavg/NMHCavg) for each ethanol composition. The linear relationship between speciationConstant parameters and ethanol composition was statistically significant for starts ($\alpha < 0.05$), but not for running emissions (Figure 3-2). Therefore, similarly to CH_4/THC ratios, we report speciationConstant parameters for start emissions (Table 3-3) at each ethanol composition analyzed, whereas for running emissions (Table 3-4) we report an average across the ethanol compositions. This approach is supported by a previous study performed by the Oak Ridge National Laboratory (ORNL)[24] which focused on the estimation of NMOG emissions from 68 vehicles using mid-level ethanol blends. The ORNL study found that given very low emissions normally measured in bag 2 and the level of scatter associated with them, the recommended approach is to use a constant NMOG/NMHC ratio across ethanol compositions.

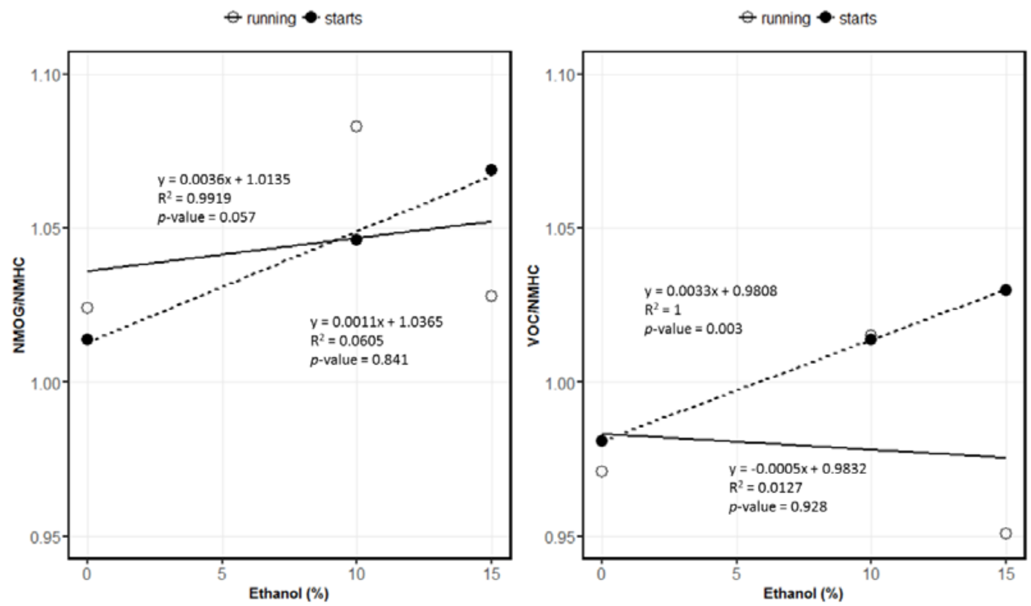

Figure 3-2 Relationship between speciationConstant Parameters and Ethanol Composition for Tier 2 Vehicles using Low-Level Ethanol Blends

Furthermore, the reported NMOG/NMHC ratio for 0 percent ethanol level in the ORNL study was 1.0302 which corresponds to the intercept of the best-fit line for the current analysis. For comparison purposes, we also determined the NMOG/NMHC ratio for the SPECIATE composite profile 8756 (Tier 2 E0 exhaust) using the methodology described in this report. The NMOG/NMHC ratio we estimated was 1.0312, showing good agreement with the value determined by the ORNL study.

Table 3-3 Updated Values CH_4/THC and speciationConstant Parameters for Start Emissions in Tier 2 Vehicles

Profile number	Profile description	Emission process	Fuel Subtype	Affected vehicles	CH_4/THC Ratio	NMOG/NMHC Ratio	VOC/NMHC Ratio
8756	Tier 2 E0 exhaust	Start exhaust and crankcase	Conventional Gasoline	2001+ LD gasoline	0.091	1.014	0.981
N/A	Tier 2 E5 exhaust	Start exhaust and crankcase	E5	2001+ LD gasoline	0.098	1.031	0.997
N/A	Tier 2 E8 exhaust	Start exhaust and crankcase	E8	2001+ LD gasoline	0.102	1.042	1.007
8757	Tier 2 E10 exhaust	Start exhaust and crankcase	E10	2001+ LD gasoline	0.105	1.046	1.014
8758	Tier 2 E15 exhaust	Start exhaust and crankcase	E15, E20	2001+ LD gasoline	0.112	1.069	1.030
8855	Tier 2 E85 exhaust	Start exhaust and crankcase	E85, E70	All gasoline vehicles running on high ethanol blends	0.273	1.511	1.454

Table 3-4 Updated CH_4/THC and speciationConstant Parameters for Running Emissions in Tier 2 Vehicles

Profile number	Profile description	Emission Process	Fuel Subtype	Affected vehicles	CH_4/THC Ratio	NMOG/NMHC Ratio	VOC/NMHC Ratio
8756	Tier 2 E0 exhaust	Running exhaust and crankcase	Conventional Gasoline	2001+ LD gasoline	0.338	1.038	0.974
N/A	Tier 2 E5 exhaust	Running exhaust and crankcase	E5	2001+ LD gasoline	0.338	1.038	0.974
N/A	Tier 2 E8 exhaust	Running exhaust and crankcase	E8	2001+ LD gasoline	0.338	1.038	0.974
8757	Tier 2 E10 exhaust	Running exhaust and crankcase	E10	2001+ LD gasoline	0.338	1.038	0.974
8758	Tier 2 E15 exhaust	Running exhaust and crankcase	E15, E20	2001+ LD gasoline	0.338	1.038	0.974
8855	Tier 2 E85 exhaust	Running exhaust and crankcase	E85, E70	All gasoline vehicles running on high ethanol blends	0.822	1.234	0.934

3.1.2.2 CNG Vehicles

The speciation values for compressed natural gas (CNG) exhaust are derived from a study conducted by the California Air Resources Board on a CNG lean-burn transit bus with and without an oxidation catalyst (Ayala et al. 2003[30]). The derivation of the CNG methane and speciationConstants are documented in Appendix B. In MOVES, we apply the speciation values from the "without control" tests to pre-2004 model year CNG vehicles, and the values "with the oxidation catalyst" to 2004 and later vehicles as shown in Table 3-5. The data used to develop the speciation constants was not complete enough to develop full speciation profiles. Thus, for purposes of speciating the residual TOG, we use SPECIATE profile 1001 (Table 4-1).

Table 3-5 CH_4/THC and speciationConstant Parameters for CNG Exhaust

Profile Description	Model Years affected	Emission process	CH_4/THC Ratio	NMOG/NMHC Ratio	VOC/NMHC Ratio
CNG lean-burn	1960-2003	Starts and running exhaust and crankcase	0.886	1.9	1.68
CNG lean-burn oxidation catalyst	2004-2060	Starts and running exhaust and crankcase	0.959	1.24	0.93

The CH_4/THC values in Table 3-5 compare well to the average methane ratios estimated from the data used to derive the THC emission rates for CNG transit buses documented in the Heavy-duty Report (0.92 for 1994-2001 model years, and 0.95 for 2002-2006 model year[25]). However, peer-reviewers of the MOVES2014 Speciation report[7] recommended we consider using more recent studies of CNG vehicles. In response, we compared the value developed from Ayala et al. (2003)[30], to more recent studies as shown in Table 3-6 which shows that the CH_4/THC value compare well with recent studies including data on stoichiometric three-way catalyst (TWC) technology engines.

Larger differences between studies are observed for the NMOG/NMHC and VOC/NMHC ratios. The differences can be explained by the fact that the CNG exhaust from Ayala et al. (2003)[30] used in MOVES contain high formaldehyde emissions, particularly for uncontrolled compression ignition buses, which causes high NMOG/NMHC ratios. The large variation in these values, may also be due to differences in measurements, particularly because non-methane hydrocarbons constitute a small fraction of the total organic gas emissions from CNG buses.

Table 3-6 Comparison of CH_4/THC and speciationConstant Parameters for CNG Engines from several studies

Study	Technology	Model year	Cycles tested	CH_4/THC Ratio	NMOG/NMHC Ratio	VOC/NMHC Ratio
CEC-2015[26]	Lean-burn	2005	CBD[a]	0.853	1.062	1.062
	Stoichiometric TWC	2011-2013	CBD	0.881	1.183	1.183
Thiruvengadam et al.[27,28]	Stoichiometric TWC	2008-2009, 2011	UDDS[b]	0.982	1.096	1.096
	Dual-Fuel High-Pressure Direct Injection (HPDI)	2011	UDDS	0.683	1.031	1.031
CE-CERT[29]	Stoichiometric TWC[c]	2014	UDDS	0.941	ND[d]	ND
	Stoichiometric TWC	2014	CBD	0.719	ND	ND
Ayala et al.[30] (MOVES)	Lean-burn, no control	2000	CBD	0.886	1.9	1.68
	Lean-burn, Oxidation catalyst	2000	CBD	0.959	1.24	0.93

Notes:
[a] Central Business District
[b] Urban Dynamometer Driving Schedule
[c] TWC= Three-way catalyst
[d] ND: Not Determined

Currently, we do not estimate evaporative or refueling emissions from CNG vehicles in MOVES and thus, have no CH_4/THC, NMOG/NMHC, and VOC/NMHC ratios for these processes. This is an area for future research.

4 Chemical Mechanism (CM) Speciation

4.1. Overview

MOVES maps the MOVES-produced components of TOG (e.g., benzene) and the remaining TOG (referred to as residual TOG or NONHAPTOG) to the CM species used by each chemical mechanism, in units of moles, for use by air-quality models. The calculation of Residual TOG is shown in Equation 10 below. In this report, this mapping process is referred to as TOG speciation.

$$\textit{Residual TOG} = \textit{TOG} - \textit{MOVES gaseous organic species} \qquad \textbf{Equation 10}$$

The MOVES gaseous organic species that are subtracted are referred to as "integrated species." Currently, we are integrating 16 MOVES species, listed in Table 2-1. The MOVES species we do not integrate are primarily the PAHs and the dioxins.

TOG speciation required for air quality models is different than PM speciation, due to the concept of chemical mechanisms. Chemical mechanisms (defined in the glossary) are used to simplify the thousands of individual organic compounds into a manageable set of CM species used for air quality modeling. The profiles used in this process, and the mapping of real species into CM species are discussed below. PM, on the other hand, is not mapped into CM species, but is split into various real species and some aggregated groups for use in air quality models (See Section 5).

4.2. Real Speciation Profiles

A real speciation profile is, in principle, a complete listing of all the real species and their quantities that make up an aggregate species such as TOG. Of course, the hundred or so compounds listed in these profiles are not a complete listing, which would likely include thousands of species. However, they are the major species by mass and reactivity. Such a profile is produced by laboratory analysis of emissions. These are not CM speciation profiles and are independent of chemical mechanism.

Table 4-1 summarizes the speciation profiles, based on SPECIATE 4.5, that we are using in MOVES, together with the fuels, affected vehicles, and MOVES emission processes to which they apply. SPECIATE is the EPA's repository of volatile organic gas and particulate matter (PM) speciation profiles from air pollution sources.[31] The Speciate Database Project began at EPA in 1988; the current version, SPECIATE 4.5, was released in September, 2016. In 2005, an EPA SPECIATE Workgroup was formed to assure inclusion of the most current data and to quality-assure the content.[32] The SPECIATE database contains a record of each profile including its referenced source, testing methods, a subjective rating of the quality of the data, and other detailed data that allow researchers to decide which profile is most suitable for model input. Table A-4 lists the referenced sources of the real speciation profiles used in MOVES.

In MOVES201X we incorporated a new speciation profile (profile ID 95335), which is based on exhaust sampling of three 2011 heavy-duty diesel engines from the ACES Phase 2 test program[23] as mentioned in Section 3.1.1.

Table 4-1. Speciation Profiles Used for Onroad TOG Emissions[c]

Profile	Profile Description	Fuel	Affected Vehicles	Emission Process
1001	CNG Exhaust	CNG	All CNG Transit Buses	Running Exhaust, Start Exhaust, Crankcase Running Exhaust, Crankcase Start Exhaust
4547	Diesel Headspace	Diesel	All Diesel	Evap Permeation, Evap Fuel Vapor Venting, Evap Fuel Leaks, Refueling Displacement Vapor Loss, Refueling Spillage Loss
8753	E0 Evap	E0	All Gas	Evap Fuel Vapor Venting, Evap Fuel Leaks, Refueling Spillage Loss
8754	E10 Evap	E10	All Gas	Evap Fuel Vapor Venting, Evap Fuel Leaks, Refueling Spillage Loss
8756	Tier 2 E0 Exhaust	E0	2001+ LD Gas	Running Exhaust, Start Exhaust, Crankcase Running Exhaust, Crankcase Start Exhaust
8757	Tier 2 E10 Exhaust	E10	2001+ LD Gas	Running Exhaust, Start Exhaust, Crankcase Running Exhaust, Crankcase Start Exhaust
8758	Tier 2 E15 Exhaust	E15, E20	All Gas	Running Exhaust, Start Exhaust, Crankcase Running Exhaust, Crankcase Start Exhaust
8766	E0 evap permeation	E0	All Gas	Evap Permeation
8769	E10 evap permeation	E10	All Gas	Evap Permeation
8770	E15 evap permeation	E15, E20	All Gas	Evap Permeation
8774	Pre-2007 MY HDD exhaust	Diesel	Pre-2007 HD Diesel	Running Exhaust, Start Exhaust, Crankcase Running Exhaust, Crankcase Start Exhaust, Crankcase Extended Idle Exhaust, Extended Idle Exhaust
8774	Pre-2007 MY HDD exhaust	Diesel	Pre-2024 APU	Auxiliary Power Exhaust
8774	Pre-2007 MY HDD exhaust	Diesel	Pre-2007 LD Diesel	Running Exhaust, Start Exhaust, Crankcase Running Exhaust, Crankcase Start Exhaust
8775	2007-2009 HDD exhaust	Diesel	2007+ LD Diesel	Running Exhaust, Start Exhaust, Crankcase Running Exhaust, Crankcase Start Exhaust
8775	2007-2009 HDD exhaust	Diesel	2007-2009 HD Diesel	Running Exhaust, Start Exhaust, Crankcase Running Exhaust, Crankcase Start Exhaust, Crankcase Extended Idle Exhaust, Extended Idle Exhaust

[c] Appendix C (Table C- 1) provides a complete mapping of the TOG speciation profiles to modelYearGroupID, processID, fuelSubTypeID, and regClassID.

Table 4-1. (continued)

Profile	Profile Description	Fuel	Affected Vehicles	Emission Process
8775	2007-2009 HDD exhaust	Diesel	2024+ APU	Auxiliary Power Exhaust
95335	2011 HDD Exhaust	Diesel	2010+ LD Diesel	Running Exhaust, Start Exhaust, Crankcase Running Exhaust, Crankcase Start Exhaust
95335	2011 HDD Exhaust	Diesel	2010+ HD Diesel	Running Exhaust, Start Exhaust, Crankcase Running Exhaust, Crankcase Start Exhaust, Crankcase Extended Idle Exhaust, Extended Idle Exhaust
8855	Tier 2 E85 Exhaust	E70, E85	E70, E85	Running Exhaust, Start Exhaust, Crankcase Running Exhaust, Crankcase Start Exhaust
8869	E0 Headspace	E0	All Gas	Refueling Displacement Vapor Loss
8870	E10 Headspace	E10	All Gas	Refueling Displacement Vapor Loss
8871	E15 Headspace	E15, E20	All Gas	Refueling Displacement Vapor Loss
8872	E15 Evap	E15, E20	All Gas	Evap Fuel Vapor Venting, Evap Fuel Leaks, Refueling Spillage Loss
8934	E85 Evap	E70, E85	E70, E85	Evap Permeation, Evap Fuel Vapor Venting, Evap Fuel Leaks, Refueling Displacement Vapor Loss, Refueling Spillage Loss
8750a	Pre-Tier 2 E0 exhaust	E0	Pre-2001 LD Gas	Running Exhaust, Start Exhaust, Crankcase Running Exhaust, Crankcase Start Exhaust
8750a	Pre-Tier 2 E0 exhaust	E0	All MC and non-LD Gas	Running Exhaust, Start Exhaust, Crankcase Running Exhaust, Crankcase Start Exhaust
8751a	Pre-Tier 2 E10 exhaust	RFG, E10	Pre-2001 LD Gas	Running Exhaust, Start Exhaust, Crankcase Running Exhaust, Crankcase Start Exhaust
8751a	Pre-Tier 2 E10 exhaust	RFG, E10	All MC and Non-LD Gas	Running Exhaust, Start Exhaust, Crankcase Running Exhaust, Crankcase Start Exhaust

4.2.1. Mapping Real Species to Chemical Mechanism Species and Residual TOG to Chemical Mechanism Speciation Profiles

The mapping of real species to CM species is mechanism-specific. Each chemical mechanism is based on a mapping of real organic gas species to one or more CM species. The atmospheric chemistry is then modeled using these CM species. CB05 and CB6CMAQ and SAPRC07T are three widely used chemical mechanisms for air quality modeling that are incorporated into MOVES201X. All the species in each real speciation profile of TOG are mapped to the chemical mechanism species associated with each chemical mechanism. Then all the occurrences of each CM species for each mechanism are added up to give molar quantities of chemical mechanism species (lumped species) for each chemical mechanism. The mappings of MOVES-generated TOG components and the residual TOG (referred to as NONHAPTOG) are generated outside of MOVES using the Speciation Tool, which converts real species profiles to CM speciation profiles.[33]

Emission estimates for species calculated directly by MOVES are based on more detailed and accurate information than those estimated using the TOG speciation profiles; therefore, we use a process called "integration" to subtract these species from the TOG speciation profiles and then develop CM speciation for the residual TOG (referred to as NONHAPTOG). For example, the benzene estimated by MOVES is based on more robust data and analysis than the benzene estimated in the TOG speciation profiles, and the same is true for the other 15 species listed in Table 2-1.To take advantage of these better data, the integration process removes the 16 pollutants from the TOG speciation profiles to produce residual-TOG speciation profiles. Then, as described above, chemical mechanism speciation profiles are produced by applying the Speciation Tool to residual-TOG.[34]

After separately mapping the integrated species and the residual TOG to CM species, MOVES adds all CM species together to produce the model-ready output of CM species. Regular MOVES output is unchanged. All chemical mechanism species are in units of moles. Because this process is table driven, MOVES201X is capable of providing CM species for multiple chemical mechanisms. Those included with this version of MOVES are CB05, CB6CMAQ, and SAPRC07T.

MOVES201X is capable of using different integrated species than the set of sixteen listed in Table 2-1. These sixteen were selected because we have high confidence that MOVES is producing more accurate results than those produced by the speciation profiles. Figure 4-3 is a diagram of the process of TOG speciation for air quality modeling.

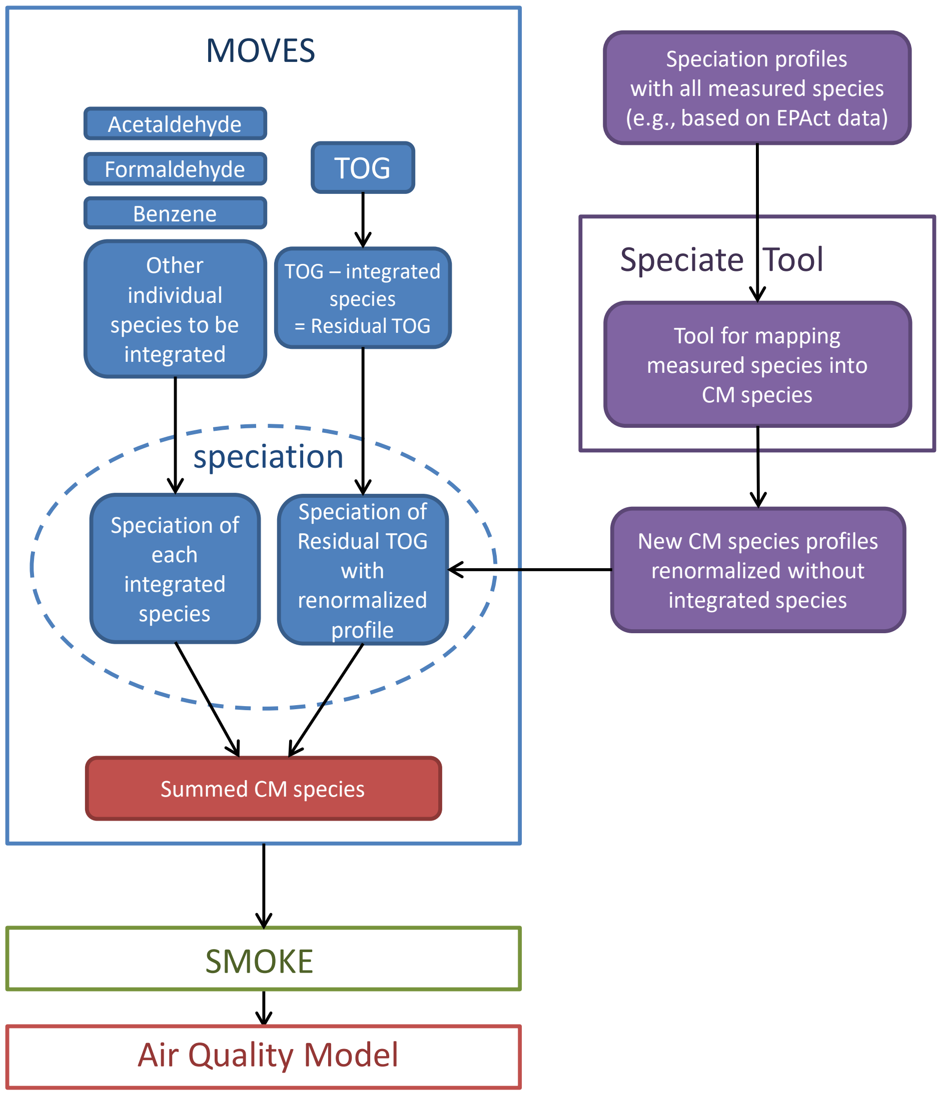

Figure 4-3. Diagram of the Process of TOG Speciation for Air Quality Modeling as it occurs with MOVES

5 $PM_{2.5}$ Speciation

Modeling $PM_{2.5}$ in CMAQ does not use simplifying chemical mechanisms, and the $PM_{2.5}$ species are input directly into the model. CMAQv5.1, which uses the CMAQ Aerosol Module, version 6, or "AE6", requires 18 $PM_{2.5}$ species as outlined in Table 5-1.[35] Theses PM species are compatible with previous versions of CMAQ and with the Comprehensive Air Quality Model with Extensions (CAMx) as shown in Table 5-1, and would be beneficial to air-quality agencies and researchers who use different air quality models. MOVES is designed to produce all $PM_{2.5}$ species required by CMAQv5.1.

Table 5-1. $PM_{2.5}$ Species Required in CMAQv5.1[d,35] and CAMx6.40[36]

$PM_{2.5}$ Species	CMAQv5.1 Species Name	Required in CAMx6.40
Primary organic carbon	POC	x
Elemental carbon	PEC	x
Sulfate	PSO4	x
Nitrate	PNO3	x
Ammonium	PNH4	x
Non-carbon organic matter	PNCOM	x
Iron	PFE	
Aluminum	PAL	
Silicon	PSI	
Titanium	PTI	
Calcium	PCA	
Magnesium	PMG	
Potassium	PK	
Manganese	PMN	
Sodium	PNA	x
Chloride	PCL	x
Particulate water	PH2O	x
Primary unspeciated $PM_{2.5}$[e]	PMOTHR	x

Similar to the methods used to speciate total organic gases, MOVES uses speciation profiles to estimate individual $PM_{2.5}$ species. The $PM_{2.5}$ Speciation profiles used are presented in Table 5-4. Although the $PM_{2.5}$ speciation data is available from the ACES Phase II Study, we are not proposing any updates to the $PM_{2.5}$ speciation profiles in MOVES201X for the reasons discussed below in Section 5.1.

[d] This version uses the CMAQ Aerosol Module, version 6, or "AE6"
[e] The definition of the unspeciated $PM_{2.5}$ depends on the set of identified $PM_{2.5}$ species in each air quality model.

5.1. $PM_{2.5}$ Speciation Calculations

Figure 5-1 and Figure 5-2 provide an overview of the algorithm used to calculate speciated and total exhaust PM emission rates in MOVES. The steps used to calculate $PM_{2.5}$ emissions and $PM_{2.5}$ speciation are outlined in nine steps below. Additional details are provided in the MOVES201X Software Design Reference Manual.[37] Steps 1 – 4 are outlined in Figure 5-1.

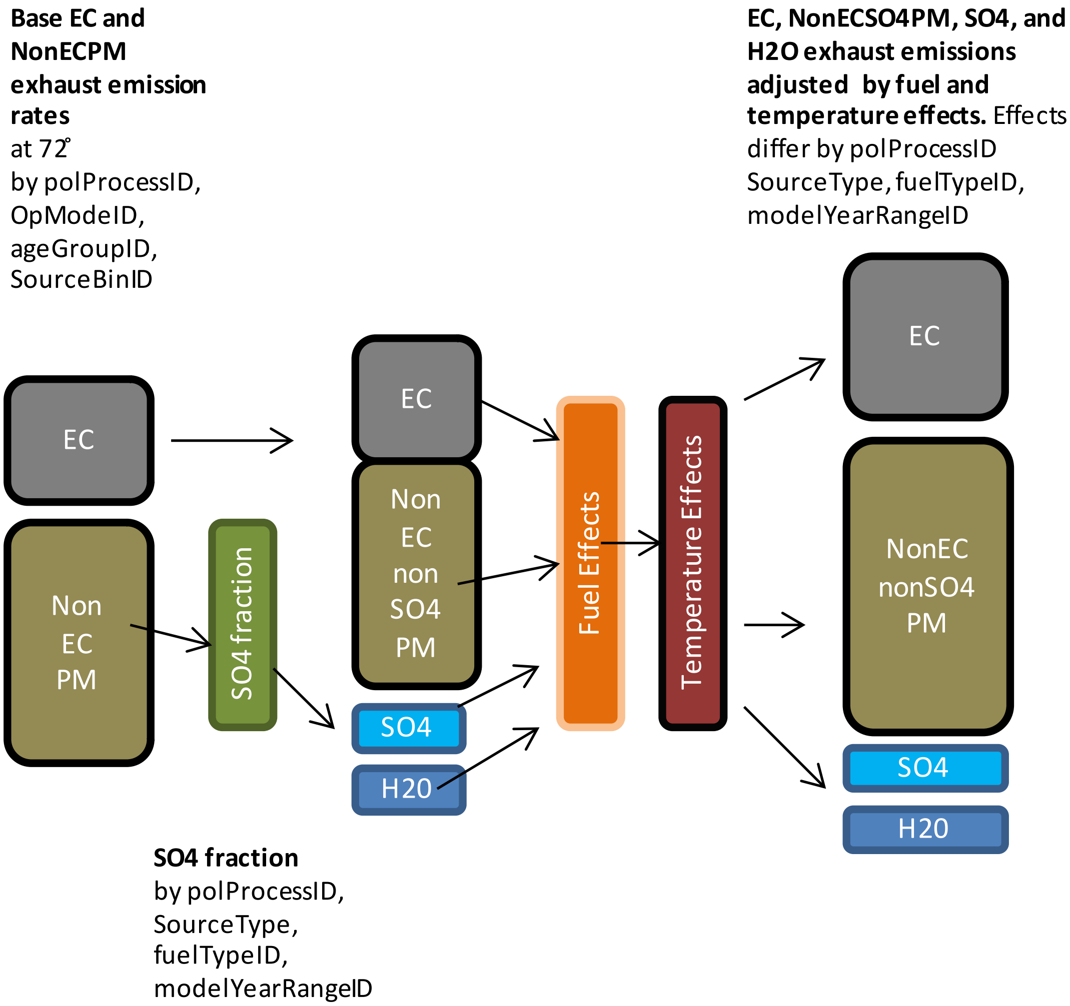

Figure 5-1. Flow Chart of Calculation of the Intermediate $PM_{2.5}$ Emission Rates

<u>Step 1.</u> MOVES stores $PM_{2.5}$ exhaust emission rates by pollutant process (start, running, extended idle), operating mode, sourcebin (fuelType, engine technology, regulatory class, model year), and vehicle age. MOVES stores the base exhaust rates for $PM_{2.5}$ in two primary components (EC and nonECPM), so that the EC/$PM_{2.5}$ ratio can vary across operating modes.[f,40]

[f] Within MOVES, modal EC/PM ratios are developed for conventional diesel vehicles (pre-2007) as documented in the Exhaust Emission Rates for Heavy-Duty On-road Vehicles in the MOVES201X Report. Modal EC/$PM_{2.5}$ ratios have not been developed for other vehicle types (gasoline, CNG, ethanol, and 2007+ diesel), and the EC and NonECPM emission rates for these sourcetypes and fuels have a constant ratio across operating modes.

Step 2. MOVES calculates sulfate (SO_4) and particulate water (H_2O) emissions as a fraction of nonECPM, using the sulfate calculator, documented in the MOVES fuel effects report.[39] The sulfate calculator adjusts the sulfate fraction based on the default or user-supplied fuel sulfur level. The remaining nonECPM is renamed nonECnonSO_4PM. This intermediate species contains organic matter, elements, ions, and the unspeciated portion of $PM_{2.5}$.

Step 3. The intermediate PM species are adjusted for temperature effects such as inefficient oxidation of emissions at cool catalyst temperatures and additional fuel needed to start an engine at cold temperatures. The temperature effects can differ by intermediate species, process (e.g. start exhaust, running exhaust, extended idle), model year groups, and fuel type. Currently, temperature effects only apply to gasoline and ethanol-blend fueled vehicles. Currently, the EC, nonECnonSO_4PM, SO_4, and H_2O emissions are each adjusted using the same temperature adjustments, because our data does not support individual temperature adjustments.[48] The temperature effects are documented in the Emission Adjustments report.[38]

Step 4. MOVES adjusts the intermediate species (EC and NonECnonSO_4PM) according to the fuel properties and the applicable fuel effects (e.g., EPAct fuel effects model for 2001 and later light-duty gasoline). The fuel adjustments and calculators are described in the Fuel Effects Report.[39]

Steps 5 – 8 are outlined in Figure 5-2.

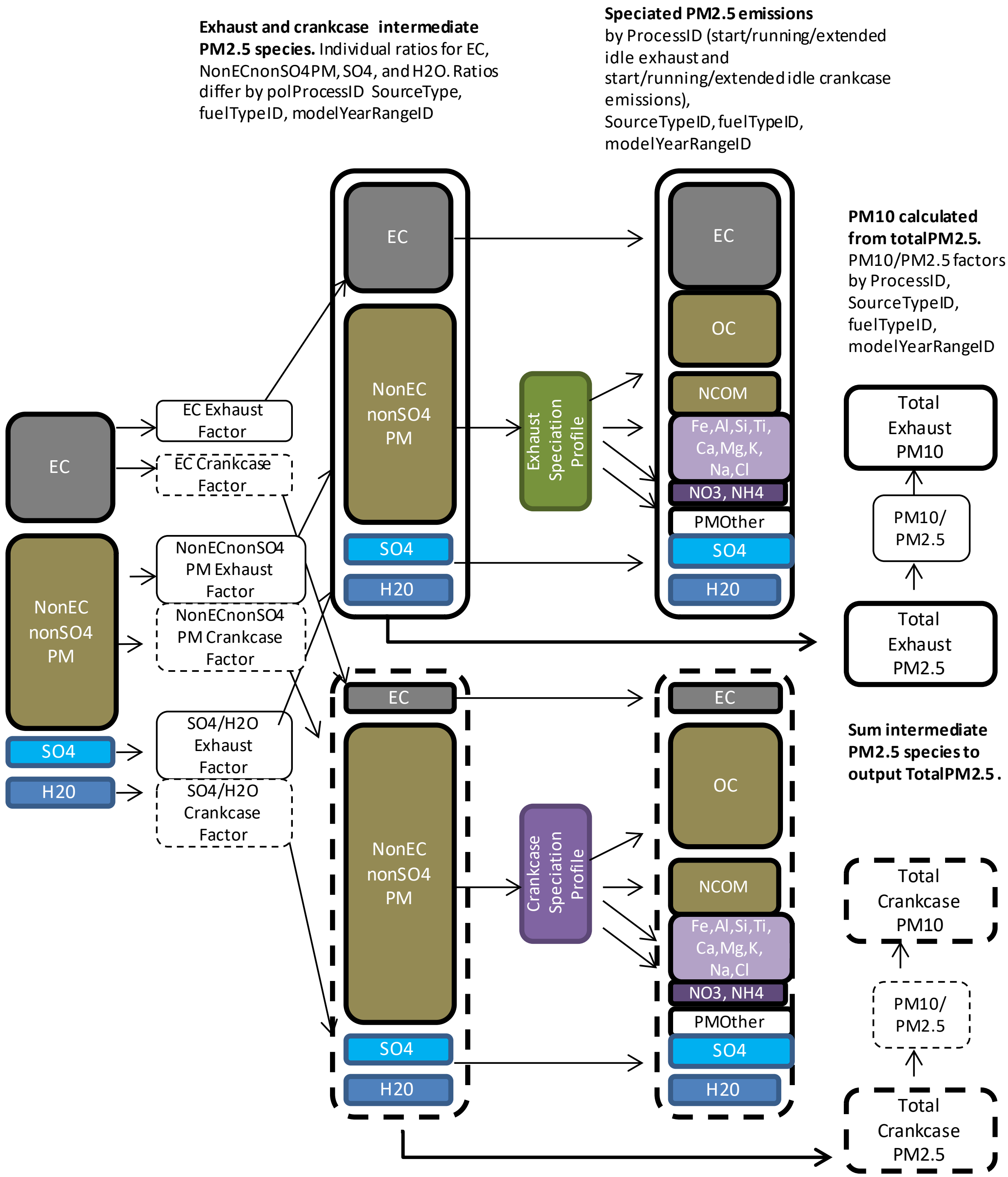

Figure 5-2. Flow Chart of Calculation of Exhaust and Crankcase $PM_{2.5}$ and PM_{10} Emission Rates, and $PM_{2.5}$ Exhaust and Crankcase Speciation

<u>Step 5.</u> Exhaust and crankcase emissions are calculated from the intermediate exhaust $PM_{2.5}$ species (EC, NonECnonSO$_4$PM, SO_4, and H_2O), after the intermediate exhaust species have been adjusted for fuel effects and temperature effects. The exhaust and crankcase emissions are

calculated from the intermediate exhaust rates with exhaust and crankcase ratios that can vary according to pollutant, process, source type, fuel type, and model year range as shown in Table 5-2.

For 2007 and later diesel engines, crankcase emissions are measured with exhaust emissions in the certification data. The exhaust and crankcase emission ratios are used to split the PM rates into exhaust and crankcase emissions. For 2007-and-later diesel, the exhaust and crankcase ratios sum to one for each PM subspecies.

For other vehicles types (pre-2007 diesel, gasoline, CNG vehicles), this step accounts for the PM crankcase emissions that are not measured in the exhaust emission rates (i.e., the exhaust and crankcase ratios sum to greater than one for each PM subspecies). The exhaust emissions remain constant in this step.

The sources of the diesel crankcase emission factors are documented in the heavy-duty exhaust emissions rates report[40] and the gasoline crankcase emission factors are documented in the light-duty exhaust emissions rates report.[41] The factors are applied by intermediate subspecies, to account for differences in $PM_{2.5}$ speciation between crankcase and tailpipe particulate matter emissions. MOVES models different PM composition between exhaust and crankcase emissions for pre-2007 conventional diesel, using the exhaust and crankcase ratios as shown in Table 5-2.

Table 5-2. Exhaust and Crankcase Ratios by Pollutant, Process, Model Year Group, and Fuel Type, and Source Type

		Motorcycles	1960-1968 Gasoline. 1960-2000 Light-Duty diesel	1960-2060 Gasoline/CNG. 2000-2060 Light-Duty diesel.	1960-2006 Heavy-Duty diesel			2007-2060 Heavy-Duty Diesel
Pollutant		All	All	All	Start	Running	Extended Idle	All
EC	Exhaust	1	1	1	1	1	1	0.62
nonEC nonSO4-PM	Exhaust	1	1	1	1	1	1	0.62
SO_4	Exhaust	1	1	1	1	1	1	0.62
H_2O	Exhaust	1	1	1	1	1	1	0.62
EC	Crankcase	0	0.2	0.008	0.009	0.004	0.012	0.38
nonEC nonSO4-PM	Crankcase	0	0.2	0.008	0.295	0.954	0.268	0.38
SO_4	Crankcase	0	0.2	0.008	0.295	0.954	0.268	0.38
H_2O	Crankcase	0	0.2	0.008	0.295	0.954	0.268	0.38

Step 6. The exhaust intermediate species and the crankcase intermediate species are summed to calculate primary exhaust $PM_{2.5}$ emissions. The intermediate species are used instead of the fully speciated $PM_{2.5}$ emissions to save computational time during MOVES runs.

Step 7. MOVES calculates primary exhaust and crankcase PM_{10} emissions from the primary $PM_{2.5}$ emissions using $PM_{10}/PM_{2.5}$ ratios. The $PM_{10}/PM_{2.5}$ ratio used for primary exhaust and crankcase emissions are listed in Table 5-3. MOVES has the capability to apply separate ratios by source type, emission process, and model year. At present, a single value of the $PM_{10}/PM_{2.5}$ ratio is used for all source types, emission processes, and model years for primary exhaust and crankcase emissions. No speciation is conducted within MOVES for PM_{10} emissions, because it is not needed for air quality modeling purposes.[g,42] The derivation of the $PM_{10}/PM_{2.5}$ ratio is presented in Appendix E.

Table 5-3 $PM_{10}/PM_{2.5}$ Ratios for Primary Exhaust and Crankcase Emissions

	$PM_{10}/PM_{2.5}$
gasoline	1.130
diesel	1.087

Step 8. MOVES calculates speciated $PM_{2.5}$ emissions, by applying speciation profiles to the adjusted nonECnonSO4 fraction to calculate the individual $PM_{2.5}$ species. The data sources and documentation for the $PM_{2.5}$ profiles are included in Table 5-4 and are also discussed in Appendix D.

Table 5-4. MOVES $PM_{2.5}$ Speciation Profiles

Profile ID	Profile Name	Source Data
8992	Light-duty Gasoline Exhaust - Start	Kansas City PM characterization Study. Final Report. EPA 420-R-08-009. U.S. EPA, April 2008. Available at: http://www.epa.gov/oms/emission-factors-research/index.htm.
8993	Light-duty Gasoline Exhaust- Hot Stabilized Running	Kansas City PM characterization Study. Final Report. EPA 420-R-08-009. U.S. EPA, April 2008. Available at: http://www.epa.gov/oms/emission-factors-research/index.htm.
8994	Conventional HDD - Idle	Clark, N.N. and Gautam, M. HEAVY-DUTY Vehicle Chassis Dynamometer Testing for Emissions Inventory, Air Quality Modeling, Source Apportionment and Air Toxics Emissions Inventory. August 2007. CRC Report. No. E55/59
8995	Conventional HDD – Hot Stabilized Running	Clark, N.N. and Gautam, M. HEAVY-DUTY Vehicle Chassis Dynamometer Testing for Emissions Inventory, Air Quality Modeling, Source Apportionment and Air Toxics Emissions Inventory. August 2007. CRC Report. No. E55/59
8996	2007 and Newer Diesel Exhaust Composite	Khalek, I. A.; Bougher, T. L; Merrit, P. M.; Phase 1 of the Advanced Collaborative Emissions Study. CRC Report: ACES Phase 1, June 2009.
95219	CNG transit bus exhaust from a lean-burn engine - no aftertreatment	Okamoto, R. A.; Kado, N. Y.; Ayala, A.; Gebel, M.; Rieger, P.; Kuzmicky, P. A.; Kobayashi, R.; Chemical and Bioassay Analyses of Emissions from Two CNG Buses with Oxidation Catalyst. http://www.arb.ca.gov/research/veh-emissions/cng-diesel/cng-diesel.htm.
95220	CNG transit bus exhaust from a lean-burn engine – oxidation catalyst	Okamoto, R. A.; Kado, N. Y.; Ayala, A.; Gebel, M.; Rieger, P.; Kuzmicky, P. A.; Kobayashi, R.; Chemical and Bioassay Analyses of Emissions from Two CNG Buses with Oxidation Catalyst. http://www.arb.ca.gov/research/veh-emissions/cng-diesel/cng-diesel.htm.

[g] Within CMAQ, the US EPA assumes a single speciation profile for all anthropogenic coarse PM.[42]

The $PM_{2.5}$ profiles used for the applicable source type, fuel, pollutant process, and model year ranges are shown in Table 5-5.

Table 5-5. Application of MOVES $PM_{2.5}$ Speciation Profiles

Profile ID	Description	Fuel	Affected Vehicles	Emission Process
8992	Light-duty Gasoline Exhaust - Start	All gasoline vehicles (E0 to E85)	All model years	Running exhaust; crankcase running exhaust.
8993	Light-duty Gasoline Exhaust- Hot Stabilized Running	All gasoline vehicles (E0 to E85)	All model years	Start exhaust; crankcase start exhaust.
8994	Conventional HDD - Idle	Diesel	Pre-2007 and all MY auxiliary power units	Running exhaust; crankcase running and extended idle exhaust; auxiliary power unit
8995	Conventional HDD – Hot Stabilized Running	Diesel	Pre-2007	Start exhaust; crankcase start exhaust.
8996	2007 and Newer Diesel Exhaust Composite	Diesel	2007+	Start exhaust; crankcase start exhaust. Running exhaust; crankcase running and extended idle exhaust; auxiliary power unit
95219	CNG transit bus exhaust from a lean-burn engine - no aftertreatment	CNG	pre-2002 model year	Start exhaust; crankcase start exhaust. Running exhaust; crankcase running and extended idle exhaust; auxiliary power unit
95220	CNG transit bus exhaust from a lean-burn engine – oxidation catalyst	CNG	2002+ model year	Start exhaust; crankcase start exhaust. Running exhaust; crankcase running and extended idle exhaust; auxiliary power unit

MOVES uses two light-duty gasoline profiles to characterize $PM_{2.5}$ emissions from all gasoline vehicles, including motorcycles, light-duty passenger cars and trucks, and medium and heavy-duty gasoline trucks and buses.

The pre-2007 diesel profiles are used to represent all pre-2007 on-highway diesel vehicles in MOVES, including light-duty passenger cars and trucks, medium, and heavy-duty trucks, and diesel buses. Tailpipe exhaust and crankcase $nonECnonSO_4$ emissions emitted during extended idle and start are speciated using the Idle Profile (8994). Tailpipe exhaust and crankcase $nonECnonSO_4$ emissions emitted during running operation are speciated using the running profile (8995). In addition, the idle profile (8994) is used to characterize $nonECnonSO_4$ emissions from diesel-powered auxiliary power units used on heavy-duty diesel trucks.

The ACES Phase 1 profile (8996) is used for all 2007-and-later diesel sources, including light-duty passenger cars and trucks, medium- and heavy-duty trucks and diesel buses. The ACES Phase 1 16-hour cycle is used to develop the profile, which includes both exhaust and crankcase emissions, as well as start, extended idle and running emission processes. For this reason, the composite profile is also used to speciate all emission processes for 2007-and-later diesel engines. It should be noted that while PM speciation data for 2010 and later diesel engines is available from the ACES Phase 2 test program, we did not update PM speciation to incorporate these data because the ACES Phase 2 emissions data did not collect any regeneration events, and thus, had minimal sulfate emissions. Testing done by California Air Resources Board[43,44] has shown regeneration events occur on 2010+ technology on-highway diesel trucks, but at a lower frequency than 2007-2009 model year trucks. During diesel particulate filter regeneration, elevated particulate matter (mostly sulfate) emissions occur, thus it is important that sulfate emissions be represented in the $PM_{2.5}$ profile.

The CNG compression ignition profile is applied to the pre-2002 model CNG heavy-duty vehicles, and the CNG profile with oxidation catalyst profile is applied to the 2002+ model year CNG heavy-duty vehicles.

Step 9. Although not shown in Figure 5-1 or Figure 5-2, MOVES can calculate additional particulate-phase species, required for the National Emission Inventory (NEI) and National Air Toxics Assessment (NATA). Listed in Table 5-6, these include: manganese, nickel, chromium, arsenic, and particulate mercury. The metals are emitted in exhaust as $PM_{2.5}$, but are calculated with a separate calculator than the other $PM_{2.5}$ species. The emission rates for these metals are not chained from $NonECSO_4PM$, but are provided with their own mass/distance rates as documented in the Air Toxic Emissions Report.[4] The mass of these compounds is not used in the summation to calculate $PM_{2.5}$ due to the very small mass, but they are important $PM_{2.5}$ exhaust species from a health effects perspective. Of the toxic metals, CMAQv5.1 only requires manganese as a required $PM_{2.5}$ species. By default, MOVES calculates manganese emission rates when the user requests $PM_{2.5}$ speciation. Chromium, nickel, arsenic, and particulate mercury emission rates are produced when requested by the user.

Table 5-6. Metal Air Toxics Produced by MOVES

Pollutant
Chromium 6+
Manganese
Nickel
Particulate Hg
Arsenic

Appendix A Supporting Information for TOG calculations

In Table A-1 and A-2, cold starts refer to the difference between bags 1 and 3. Running data corresponds to stabilized emissions from bag 2. In the particular case of running emissions, seven tests (shown in grey in Table A-1 and A-2) were not considered in the analysis because the reported CH_4 emissions were higher than the reported THC emissions, possibly because measurements were close to the detection limit of the instrument.

Table A-1 Data[h] Used to Generate CH_4/THC Ratios for Tier 2 Vehicles Running on Low-Level Ethanol Blends

SPECIATE Profile	Run Number EPAct Phase 1	Ethanol (%)	Bag1 – Bag 3		Bag 2	
			CH_4 (g/mi)	THC (g/mi)	CH_4 (g/mi)	THC (g/mi)
8756	3162	0	0.047847	0.427396	0.005536	0.016363
	3169	0	0.04971	0.569501	0.00559	0.017147
	3179	0	0.024225	0.298518	0.000759	1.43E-05
	3190	0	0.026548	0.355495	0.000677	0
	3205	0	0.042478	0.368635	0.006478	0.024158
	3215	0	0.042606	0.430156	0.006192	0.025502
	3223	0	0.018577	0.235636	0.000715	0.001726
	3231	0	0.016709	0.210923	0.000813	0.00422
	3239	0	0.030034	0.382012	0.000571	0.000311
8757	3280	10	0.031025	0.351082	0.000768	0
	3291	10	0.02948	0.343357	0.000882	0.001396
	3302	10	0.044792	0.362164	0.004702	0.014283
	3313	10	0.049488	0.382168	0.005731	0.021492
	3326	10	0.015571	0.163023	0.000793	0.003561
	3339	10	0.016341	0.164704	0.000647	0.003404
8758	3480	15	0.058352	0.448346	0.006899	0.017882
	3492	15	0.053022	0.423568	0.007144	0.014217
	3508	15	0.016634	0.140505	0.000786	0.001563
	3516	15	0.017372	0.208814	0.000774	0.001745
	3542	15	0.052195	0.493528	0.000877	0
	3553	15	0.042834	0.378627	0.001061	0
	3568	15	0.021715	0.247811	0.000963	0

[h] Data for the EPAct Phase 1 program can be found at EPA-HQ-OAR-2011-0135-2181.

Table A-2 Data[i] used to Generate speciationConstant Parameters for Tier 2 Vehicles Running on Low-Level Ethanol Blends

SPECIATE Profile	Run Number EPAct Phase 1	Ethanol (%)	Cold Start NMOG (g/mi)	Cold Start VOC (g/mi)	Cold Start NMHC (g/mi)	Running NMOG (g/mi)	Running VOC (g/mi)	Running NMHC (g/mi)
8756	3162	0	0.34466	0.33162	0.338208	0.00858	0.00806	0.008373
	3169	0	0.4684	0.45323	0.457907	0.01016	0.00961	0.00985
	3179	0	0.25556	0.24967	0.254602	0.00118	0.00113	0.001167
	3190	0	0.28376	0.27591	0.282205	0.0007	0.00058	0.000616
	3205	0	0.31373	0.30102	0.30579	0.01297	0.01227	0.012903
	3215	0	0.35952	0.34597	0.353327	0.01258	0.01197	0.01253
	3223	0	0.19666	0.18985	0.195655	0.00084	0.00078	0.00076
	3231	0	0.16773	0.16189	0.165441	0.00397	0.00393	0.003553
	3239	0	0.29545	0.28707	0.294026	0.00082	0.00076	0.000809
8757	3280	10	0.3121	0.3048	0.301382	0.0011	0.0011	0.000661
	3291	10	0.3145	0.3056	0.300919	0.0001	0.0001	0.0001
	3302	10	0.3312	0.3203	0.316833	0.0066	0.0061	0.006016
	3313	10	0.3445	0.3319	0.327144	0.0076	0.0071	0.0074
	3326	10	0.1443	0.1392	0.137216	0.0003	0.0003	0.0003
	3339	10	0.1589	0.1535	0.150808	0.0002	0.0002	0.0002
8758	3480	15	0.3897	0.3723	0.362817	0.0118	0.0108	0.0115
	3492	15	0.3706	0.3544	0.348353	0.012	0.0111	0.0117
	3508	15	0.1432	0.1373	0.132605	0.0012	0.0012	0.0012
	3516	15	0.1879	0.1822	0.172205	0	0	0
	3542	15	0.433	0.4197	0.409536	0.0004	0.0004	0.0003
	3553	15	0.3282	0.3171	0.309834	0	0	0
	3568	15	0.2387	0.2318	0.221149	0	0	0

Table A-3 documents the CH_4/THC and speciationConstant parameters for all the sources in MOVES (by including the data from Table 3-2, Table 3-3, Table 3-4, and Table 3-5). In addition, it specifies the MOVES variables that are used to define the CH4/THC and speciationConstants within the MethaneTHCRatio and HcSpeciation tables, respectively.

[i] Data for the EPAct Phase 1 program can be found at EPA-HQ-OAR-2011-0135-2181.

Table A-3 Updated CH_4/THC and speciationConstant Parameters and Their Relationship to MOVES Variables

Profile number	Profile description	modelYear-GroupID	processID	fuelSubType ID	regClassID	CH_4/THC	NMOG/NMHC	VOC/NMHC
4547	Diesel headspace	19602060	11	20,21,22	0	0	1	1
			12,13,18,19	20,21,22	10,20,30,40,41,42,46,47,48			
8750a	Pre-Tier 2 E0 exhaust	19602000	1,2,15,16	10	20,30	0.142	1.024	0.996
		19602060			10,40,41,42,46,47,48			
8751a	Pre-Tier 2 E10 exhaust	19602000	1,2,15,16	11,12,13,14	20,30	0.146	1.037	1.008
		19602060			10,40,41,42,46,47,48			
8753	E0 Evap	19602060	12,13,19	10	10,20,30,40,41,42,46,47,48	0	1	1
8754	E10 Evap	19602060	12,13,19	12,13,14	10,20,30,40,41,42,46,47,48	0	1.071	1.071
8766	E0 Evap perm	19602060	11	10	0	0	1	1
8769	E10 Evap perm	19602060	11	12,13,14	0	0	1.129	1.129
8770	E15 Evap perm	19602060	11	15,18	0	0	1.175	1.175
8774	Pre-2007 MY HDD exhaust	19602006	1,2,15,16,17,90	20,21,22	40,41,42,46,47,48	0	1.145	1.124
		19602023	91		46,47			
		19602006	1,2,15,16		20,30			
8775	2007-2009 HDD exhaust	20072009	1,2,15,16	20,21,22	20,30	0.589	1.343	1.285
		2024-2060	91		47,48			
		2007-2009	1,2,15,16,17,90		40,41,42,46,47,48			
9335	2010+ HDD exhaust	20102060	1,2,15,16	20,21,22	20, 30	0	1.085	0.965
			1,2,15,16,17,90		40,41,42,46,47,48			

Table A-3. (continued)

Profile number	Profile description	modelYear GroupID	processID	fuelSubType ID	regClassID	CH_4/THC	NMOG/NMHC	VOC/NMHC
8869	E0 Headspace	19602060	18	10	10,20,30,40,41,42,46,47,48	0	1	1
8870	E10 Headspace	19602060	18	12,13,14	10,20,30,40,41,42,46,47,48	0	1	1
8871	E15 Headspace	19602060	18	15,18	10,20,30,40,41,42,46,47,48	0	1	1
8872	E15 Evap	19602060	12,13,19	15,18	10,20,30,40,41,42,46,47,48	0	1.118	1.118
8934	E85 Evap	19602060	11	50,51,52	10,20,30,40	0	1.501	1.501
			12,13,18,19		10,20,30,40			

Table A-4 Data Sources for the MOVES Profiles

Profile ID	Profile Name	Source Data	Additional Documentation
1001	Internal Combustion Engine - Natural Gas	Oliver, W. R. and S. H. Peoples, Improvement of the Emission Inventory for Reactive Organic Gases and Oxides of Nitrogen in the South Coast Air Basin, Volumes I and II, Final Report (Prepared for California Air Resources Board), May 1985.	
4547	Gasoline Headspace Vapor - Circle K Diesel - adjusted for oxygenates	Internal data collection effort, Charles Lewis, U.S. EPA Office of Research and Development, with Ying Hsu, E.H. Pechan & Associates, Inc., personal communication (t), June 29, 2004.	SPECIATE 4.5. SPECIATE Version 4.5 Database Development Documentation No. EPA/600-R-16/294, U.S. EPA, September 2016. Available at: https://www.epa.gov/air-emissions-modeling/speciate-version-45-through-40
8750a	Gasoline Exhaust - Reformulated gasoline (pre-Tier 2)	Kansas City PM characterization Study. Final Report. EPA 420-R-08-009. U.S. EPA, April 2008. Available at: http://www.epa.gov/oms/emission-factors-research/index.htm.	Emission Profiles for EPA SPECIATE Database. EPA Contract No. EP-C-06-094. Environ Corporation, January 2008. Available at: http://www.regulations.gov. Docket ID: EPA-HQ-OAR-2005-0161, Document ID: EPA-HQ-OAR-2005-0161-2710.
8751a	Gasoline Exhaust - E10 ethanol gasoline (pre-Tier 2)	Kansas City PM characterization Study. Final Report. EPA 420-R-08-009. U.S. EPA, April 2008. Available at: http://www.epa.gov/oms/emission-factors-research/index.htm.	Emission Profiles for EPA SPECIATE Database. EPA Contract No. EP-C-06-094. Environ Corporation, January 2008. Available at: http://www.regulations.gov. Docket ID: EPA-HQ-OAR-2005-0161, Document ID: EPA-HQ-OAR-2005-0161-2710.
8753	Gasoline Vehicle - Evaporative emission - Reformulated gasoline	Auto/Oil Air Quality Improvement Research Program. Coordinating Research Council, 1990-1997. List of reports at: http://www.crcao.com/reports/auto-oil/default.htm	Emission Profiles for EPA SPECIATE Database. EPA Contract No. EP-C-06-094. Environ Corporation, January 2008. Available at: http://www.regulations.gov. Docket ID: EPA-HQ-OAR-2005-0161, Document ID: EPA-HQ-OAR-2005-0161-2710.
8754	Gasoline Vehicle - Evaporative emission - E10 ethanol gasoline	Auto/Oil Air Quality Improvement Research Program. Coordinating Research Council, 1990-1997. List of reports at: http://www.crcao.com/reports/auto-oil/default.htm	Emission Profiles for EPA SPECIATE Database. EPA Contract No. EP-C-06-094. Environ Corporation, January 2008. Available at: http://www.regulations.gov. Docket ID: EPA-HQ-OAR-2005-0161, Document ID: EPA-HQ-OAR-2005-0161-2710.
8756	Gasoline Exhaust - Tier 2 light-duty vehicles using 0% Ethanol - Composite Profile	Data Collected in EPAct Fuel Effects Study Pilot Phases 1 and 2. Memorandum to the Tier 3 Docket. U.S. EPA, 2013 Available at: http://www.regulations.gov. Docket ID: EPA-HQ-OAR-2011-0135.	Exhaust Emission Profiles for EPA SPECIATE Database: Energy Policy Act (EPAct) Low-Level Ethanol Fuel Blends and Tier 2 Light-Duty Vehicles. EPA Report No. EPA-420-R-09-002. U.S. EPA, 2009. Available at: http://www.regulations.gov. Docket ID: EPA-HQ-OAR-2005-0161, Document ID: EPA-HQ-OAR-2005-0161-2711.
8757	Gasoline Exhaust - Tier 2 light-duty vehicles using 10% Ethanol - Composite Profile	Data Collected in EPAct Fuel Effects Study Pilot Phases 1 and 2. Memorandum to the Tier 3 Docket. U.S. EPA, 2013 Available at: http://www.regulations.gov. Docket ID: EPA-HQ-OAR-2011-0135.	Exhaust Emission Profiles for EPA SPECIATE Database: Energy Policy Act (EPAct) Low-Level Ethanol Fuel Blends and Tier 2 Light-Duty Vehicles. EPA Report No. EPA-420-R-09-002. U.S. EPA, 2009. Available at: http://www.regulations.gov. Docket ID: EPA-HQ-OAR-2005-0161, Document ID: EPA-HQ-OAR-2005-0161-2711.
8758	Gasoline Exhaust - Tier 2 light-duty vehicles using 15% Ethanol - Composite Profile	Data Collected in EPAct Fuel Effects Study Pilot Phases 1 and 2. Memorandum to the Tier 3 Docket. U.S. EPA, 2013 Available at: http://www.regulations.gov. Docket ID: EPA-HQ-OAR-2011-0135.	Exhaust Emission Profiles for EPA SPECIATE Database: Energy Policy Act (EPAct) Low-Level Ethanol Fuel Blends and Tier 2 Light-Duty Vehicles. EPA Report No. EPA-420-R-09-002. U.S. EPA, 2009. Available at: http://www.regulations.gov. Docket ID: EPA-HQ-OAR-2005-0161, Document ID: EPA-HQ-OAR-2005-0161-2711.

Table A-4. (continued)

Profile ID	Profile Name	Source Data	Additional Documentation
8766	Diurnal Permeation Evaporative Emissions from Gasoline Vehicles using 0% Ethanol - Combined - Composite Profile	Evaporative Emissions from In-use Vehicles: Test Fleet Expansion. CRC E-77-2b. SWRI Project No. 03.14936.05. Final report. Available at: http://www.epa.gov/otaq/emission-factors-research/	
8769	Diurnal Permeation Evaporative Emissions from Gasoline Vehicles using 10% Ethanol - Combined - Composite Profile	Evaporative Emissions from In-use Vehicles: Test Fleet Expansion. CRC E-77-2b. SWRI Project No. 03.14936.05. Final report. Available at: http://www.epa.gov/otaq/emission-factors-research/	
8770	Diurnal Permeation Evaporative Emissions from Gasoline Vehicles using 15% Ethanol - Combined	Evaporative Emissions from In-use Vehicles: Test Fleet Expansion. CRC E-77-2b. SWRI Project No. 03.14936.05. Final report. Available at: http://www.epa.gov/otaq/emission-factors-research/	
8774	Diesel Exhaust Emissions from Pre-2007 Model Year Heavy-Duty Diesel Trucks	Heavy-duty Vehicle Chassis Dynamometer Testing for Emissions Inventory, Air Quality Modeling, Source Appointment and Air Toxics Emissions Inventory. CRC Project No. E-55/E-59, Phase II Final Report. Coordinating Research Council, July 2005. Available at: http://www.crcao.com/publications/emissions/index.html	
8775	Diesel Exhaust Emissions from 2007 Model Year Heavy-Duty Diesel Engines with Controls	Phase 1 of the Advanced Collaborative Emissions Study. Coordinating Research Council, July 2009. Available at: http://www.crcao.com/publications/emissions/index.html	
8855	Gasoline Exhaust - Tier 2 light-duty vehicles using 85% Ethanol - Composite Profile	EPAct/V2/E-89: Assessing the Effect of Five Gasoline Properties on Exhaust Emissions from Light-Duty Vehicles Certified to Tier-2 Standards: Final Report on Program Design and Data Collection. EPA-420-R-13-004. U.S. EPA, April 2013. Available at: http://www.epa.gov/otaq/models/moves/epact.htm.	
8869	Gasoline Headspace Vapor - 0% Ethanol (E0) Combined - EPAct/V2/E-89 Program	Hydrocarbon Composition of Gasoline Vapor Emissions from Enclosed Fuel Tanks, Report No. 420-R-11-018. U.S. EPA, December 2011. Available at: http://www.regulations.gov, Docket ID: EPA-HQ-OAR-2011-0135, Document ID: EPA-HQ-OAR-2011-0135-0027.	Mobile Source Hydrocarbon Speciation Profiles for the Tier 3 Rule NPRM and Anti-backsliding Study Air Quality Modeling. Memorandum to the Docket. U.S. EPA, 2013. Available at: http://www.regulations.gov. Docket ID: EPA-HQ-OAR-2011-0135, Document ID: EPA-HQ-OAR-2011-0135-0089.

Table A-4. (continued)

Profile ID	Profile Name	Source Data	Additional Documentation
8870	Gasoline Headspace Vapor - 10% Ethanol (E10) Combined - EPAct/V2/E-89 Program	Hydrocarbon Composition of Gasoline Vapor Emissions from Enclosed Fuel Tanks, Report No. 420-R-11-018. U.S. EPA, December 2011. Available at: http://www.regulations.gov, Docket ID: EPA-HQ-OAR-2011-0135, Document ID: EPA-HQ-OAR-2011-0135-0027.	Mobile Source Hydrocarbon Speciation Profiles for the Tier 3 Rule NPRM and Anti-backsliding Study Air Quality Modeling. Memorandum to the Docket. U.S. EPA, 2013. Available at: http://www.regulations.gov. Docket ID: EPA-HQ-OAR-2011-0135, Document ID: EPA-HQ-OAR-2011-0135-0089.
8871	Gasoline Headspace Vapor - 15% Ethanol (E15) Combined - EPAct/V2/E-89 Program	Hydrocarbon Composition of Gasoline Vapor Emissions from Enclosed Fuel Tanks, Report No. 420-R-11-018. U.S. EPA, December 2011. Available at: http://www.regulations.gov, Docket ID: EPA-HQ-OAR-2011-0135, Document ID: EPA-HQ-OAR-2011-0135-0027.	Mobile Source Hydrocarbon Speciation Profiles for the Tier 3 Rule NPRM and Anti-backsliding Study Air Quality Modeling. Memorandum to the Docket. U.S. EPA, 2013. Available at: http://www.regulations.gov. Docket ID: EPA-HQ-OAR-2011-0135, Document ID: EPA-HQ-OAR-2011-0135-0089.
8872	Gasoline Vehicle - Evaporative emission - E15 ethanol gasoline - Calculated	Auto/Oil Air Quality Improvement Research Program. Coordinating Research Council, 1990-1997. List of reports at: http://www.crcao.com/reports/auto-oil/default.htm EPAct/V2/E-89: Assessing the Effect of Five Gasoline Properties on Exhaust Emissions from Light-Duty Vehicles Certified to Tier-2 Standards: Final Report on Program Design and Data Collection. EPA-420-R-13-004. U.S. EPA, April 2013. Available at: http://www.epa.gov/otaq/models/moves/epact.htm.	Mobile Source Hydrocarbon Speciation Profiles for the Tier 3 Rule NPRM and Anti-backsliding Study Air Quality Modeling. Memorandum to the Docket. U.S. EPA, 2013. Available at: http://www.regulations.gov. Docket ID: EPA-HQ-OAR-2011-0135, Document ID: EPA-HQ-OAR-2011-0135-0089.
8934	Evaporative Emissions from Flexible-Fuel Gasoline Vehicles using 85% Ethanol	Exhaust and Evaporative Emissions Testing of Flexible-Fuel Vehicles. Final report. CRC Report CRC-E-80. Coordinating Research Council, Inc. August 2011. Report and program data available at http://www.crcao.org/publications/emissions/index.html	
9335	Diesel Exhaust – Heavy-heavy duty truck – 2011 model year	Khalek, I., Blanks, M., and Merritt, P. M. (2013). Phase 2 of the Advanced Collaborative Emissions Study. Prepared by Southwest Research Institute for the Coordinating Research Council and the Health Effects Institute, November 2013. Available at www.crcao.org.	

Appendix B CNG CH_4/THC and speciationConstant parameters for CNG vehicles

SPECIATE does not contain a TOG speciation profile from modern CNG exhaust emissions. We used hydrocarbon speciation data from Ayala et al. that measured a 2000 MY transit bus with a Detroit Diesel Series 50G engine with and without an oxidation catalyst collected on the CBD cycle.[30] This data allows us to isolate the impact of the oxidation catalyst. Studies have shown that the speciation of hydrocarbon can be drastically different between uncontrolled CNG buses and CNG buses with oxidation catalysts. For example, formaldehyde emissions can be quite large from uncontrolled CNG buses[45,46], but are significantly reduced with oxidation catalysts.[30] Large formaldehyde emissions have a large impact on the NMOG and VOC emissions estimated from THC emissions from CNG buses because THC-FID measurements have a small response to formaldehyde concentrations.[47]

We used the CBD test cycle to be consistent with our analysis of the criteria emission rates documented in the heavy-duty emission rate report.[40] The NMOG and VOC conversion factors are listed in Table B-1. The NMOG values are calculated using Equation 7. The VOC emissions are calculated from subtracting the ethane and acetone from the NMOG values. The emissions of hazardous air pollutants, including formaldehyde and acetaldehyde, are also estimated from this study as documented in the MOVES201X Toxics Emissions Report.[4]

Table B-1 Hydrocarbon Speciation Values for CNG Transit Emissions with No Control and with Oxidation Catalyst from Ayala et al. (2003)[30]

Measured values (mg/mile)	No Control	Oxidation Catalyst
THC	8660	6150
CH4	7670	5900
C2H6	217	72.2
Formaldehyde	860	38.4
Acetaldehyde	50.7	32.6
Calculated values (mg/mile)		
NMHC	990	250
NMOG	1881.0	309.0
VOC	1658.5	232.1
Ratios		
NMOG/NMHC	1.90	1.24
VOC/NMHC	1.68	0.93

Appendix C TOG Speciation Map

Table C-1provides a complete speciation map between MOVES profiles and the distinguishing factors used in MOVES: modelYearGroupID, processID, fuelSubTypeID, and regClassID.

Table C-1 TOG Speciation Map

Profile	Profile Description	modelYear-GroupID	processID	fuelSubTypeID	regClassID
1001	CNG Exhaust	19602060	1,2,15,16	30	48
4547	Diesel Headspace	19602060	11	20,21,22	0
4547	Diesel Headspace	19602060	12,13,18,19	20,21,22	10,20,30,40,41,42,46,47,48
8753	E0 Evap	19602060	12,13,19	10	10,20,30,40,41,42,46,47,48
8754	E10 Evap	19602060	12,13,19	12,13,14	10,20,30,40,41,42,46,47,48
8756	Tier 2 E0 Exhaust	20012060	1,2,15,16	10	20,30
8757	Tier 2 E10 Exhaust	20012060	1,2,15,16	12,13,14	20,30
8758	Tier 2 E15 Exhaus	19602060	1,2,15,16	15,18	10,20,30,40,41,42,46,47,48
8766	E0 evap permeation	19602060	11	10	0
8769	E10 evap permeation	19602060	11	12,13,14	0
8770	E15 evap permeation	19602060	11	15,18	0
8774	Pre-2007 MY HDD exhaust	19602006	1,2,15,16,17,90	20,21,22	40,41,42,46,47,48
8774	Pre-2007 MY HDD exhaust	19602060	91	20,21,22	46,47
8774	Pre-2007 MY HDD exhaust	19602006	1,2,15,16	20,21,22	20,30
8775	2007+ MY HDD exhaust	20072009	1,2,15,16	20,21,22	20,30
8775	2007+ MY HDD exhaust	20072009	1,2,15,16,17,90	20,21,22	40,41,42,46,47,48
9335	2010+ MY HDD exhaust	20102060	1,2,15,16	20,21,22	20,30
9335	2010+ MY HDD exhaust	20102060	1,2,15,16,17,90	20,21,22	40,41,42,46,47,48
8855	Tier 2 E85 Exhaust	19602060	1,2,15,16	50,51,52	10,20,30,40,41,42,46,47,48
8869	E0 Headspace	19602060	18	10	10,20,30,40,41,42,46,47,48
8870	E10 Headspace	19602060	18	12,13,14	10,20,30,40,41,42,46,47,48
8871	E15 Headspace	19602060	18	15,18	10,20,30,40,41,42,46,47,48
8872	E15 Evap	19602060	12,13,19	15,18	10,20,30,40,41,42,46,47,48
8934	E85 Evap	19602060	11	50,51,52	0

Table C-1. (continued)

Profile	Profile Description	modelYear-GroupID	processID	fuelSubTypeID	regClassID
8934	E85 Evap	19602060	12,13,18,19	50,51,52	20,30,40
8750a	Pre-Tier 2 E0 exhaust	19602000	1,2,15,16	10	20,30
8750a	Pre-Tier 2 E0 exhaust	19602060	1,2,15,16	10	10,40,41,42,46,47,48
8751a	Pre-Tier 2 E10 exhaust	19602000	1,2,15,16	11,12,13,14	20,30
8751a	Pre-Tier 2 E10 exhaust	19602060	1,2,15,16	11,12,13,14	10,40,41,42,46,47,48

Appendix D Development of $PM_{2.5}$ speciation profiles in MOVES

This report includes the derivation of each $PM_{2.5}$ profiles used in MOVES.

For comparison purposes, the seven $PM_{2.5}$ profiles developed for MOVES are presented in Table D-1. In the following subsections, the analyses to derive each of these profiles are presented.

Table D-1 $PM_{2.5}$ Profiles developed for MOVES

	Light-duty Gasoline Exhaust – Start (8992)	Light-duty Gasoline Exhaust- Hot Stabilized (8993)	Conventional HDD- Idle (8994)	Conventional HDD- Hot Stabilized Running (8995)	2007 and Newer Diesel Exhaust Composite (8996)	CNG transit bus exhaust from a lean-burn engine - no aftertreatment (95219)	CNG transit bus exhaust from a lean-burn engine - no aftertreatment (95220)
Elemental Carbon (EC)	44.37%	14.00%	46.40%	78.97%	9.98%	9.25%	11.12%
Organic Carbon (OC)	42.64%	55.70%	34.74%	14.52%	22.33%	36.99%	37.45%
Non-carbon Organic Matter (NCOM)	8.53%	11.14%	6.95%	2.90%	4.47%	7.40%	7.49%
SO4	0.95%	7.19%	5.27%	1.03%	59.91%	0.64%	1.04%
NO3	0.26%	0.29%	1.25%	0.18%	0.00%		
NH4	0.43%	2.78%	1.74%	0.36%	0.00%		
Fe	0.31%	1.83%	0.34%	0.13%	0.64%	0.25%	0.25%
Al		0.32%	0.06%	0.06%	0.11%	0.89%	0.89%
Si		0.32%	0.30%	0.22%	0.09%	0.46%	0.59%
Ti		0.03%	0.01%	0.01%	0.02%		
Ca	0.39%	1.44%	0.58%	0.35%	0.47%	0.21%	0.44%
Mg	0.02%	0.14%	0.13%	0.01%	0.14%		
K		0.09%	0.26%	0.02%	0.05%		
Na	0.01%	0.04%	0.31%	0.03%	0.99%		
Cl	0.02%	0.10%	0.38%	0.13%	0.04%		
unspeciated (PMOTHR)	2.09%	4.58%	1.28%	1.09%	0.78%	43.90%	40.74%

D.1 *Development of Gasoline Profiles from the Kansas City Light-duty Vehicle Emissions Study*

The Kansas City Light-duty Vehicle Emissions Study (KCVES) is the primary source of $PM_{2.5}$ emission rates for light-duty vehicles in MOVES.[41] The KCVES sampled $PM_{2.5}$ emissions from 496 vehicles recruited in a stratified random sample. The KCVES also measured speciated $PM_{2.5}$ on a subset of 99 of these vehicles. An overview of the vehicles included in the chemical subset is included in Table D-2.

Table D-2 Vehicle Sample Size in the Kansas City Light Duty Vehicle Emissions Study

Vehicle Type[1]	Strata	Model Year Group	% of KC LDGV Vehicle Population	% of KC LDGV Vehicle Miles Traveled (VMT)	Summer Round Sample		Winter Round Sample	
					Full Sample	Chemical Subset	Full Sample	Chemical Subset
Truck	1	pre-1981	1.1%	0.6%	2	2	10	3
	2	81-90	3.7%	2.4%	21	4	33	3
	3	91-95	7.2%	6.5%	18	6	33	7
	4	96-2005	28.6%	34.2%	39	8	59	11
Car	5	pre-1981	1.3%	0.7%	6	5	17	3
	6	81-90	7.4%	4.6%	49	4	40	5
	7	91-95	13.4%	11.2%	39	6	44	9
	8	96-2005	37.3%	39.8%	87	14	41	9
		Sum =	100%	100%	261	49	277	50

The derivation of the $PM_{2.5}$ gasoline profile for MOVES is documented in Sonntag *et al.* (2013).[48] A summary of the speciation derivation is included in this report, as well as a discussion on implementing the profile into the MOVES framework. Two gasoline profiles are developed to maintain differences between start and running processes. Minor differences were detected between the $PM_{2.5}$ compositions between seasons, which were confounded by the different vehicles tested in each season. The data used equally weighted data from the summer and winter tests to calculate a profile that incorporates data from both seasons.

We discovered high concentrations of silicon in some of the $PM_{2.5}$ measurements, likely due to contamination from silicone rubber couplers used in KCVES. The silicone contamination occurred primarily on bag 2 of the LA-92 drive cycle which was used for developing the running $PM_{2.5}$ speciation profile and emission rates. The silicone contamination was larger for trucks than cars due to their higher exhaust temperatures. The effect of the silicone contamination was removed from the developed profile using the silicon emissions measurement by X-ray florescence. The primary exhaust $PM_{2.5}$ emission rates were corrected in MOVES to account for the silicone contamination.[41] After removing the silicone contamination from the speciated data, no significant differences were detected between passenger cars and light-duty trucks, and the data from the cars and trucks were pooled together to develop single start and running $PM_{2.5}$ speciation profiles for all light-duty gasoline vehicles.

Important differences in the $PM_{2.5}$ compositions were detected among model year groups. Rather than calculating model-year-group-specific profiles, fleet-average profiles were calculated to better capture the impact of deterioration within all model year groups and to avoid over-fitting the data to model year group trends. Malfunctioning high-emitting vehicles are known to contribute a significant share of in-use PM emissions from light-duty vehicles.[49,50,51,52] High-emitting gasoline emissions have a highly variable PM composition due to failed emission control systems, excessive oil consumption, and poor fuel control. Previous analysis of the KCVES suggested that the speciation subsample (102 tests) provides a reasonable estimate of the total PM mass compared to the full sample (522 tests), but the speciation sample underestimated the high emitting vehicles in the newer model year groups.[53] Other test programs have confirmed that high emitting gasoline vehicles also occur in modern vehicle fleets such as 1990-era vehicles with electronic fuel injection.[49,50,51] The speciation sample size was deemed too limited to accurately capture the impact of deterioration and high-emitting vehicles within each model-year group. By using all the data in a fleet-average approach, we incorporated the impact of deteriorated vehicles on the fleet-average $PM_{2.5}$ emissions.

The fleet-average PM speciation profiles are calculated using seasonal, vehicle-miles-traveled (VMT), and PM mass-weighting. The PM profile is calculated using the ratio of the means, also referred to as a mass-normalized emission profile.[54] The ratio of means is calculated by first calculating the mean emission rate of the total $PM_{2.5}$, and the mean emission rate of each PM species (EC, OC, Fe, etc.). Then the speciation profile is calculated, by calculating the ratio of the mean emission rate from each species, to the mean $PM_{2.5}$ emission rate, e.g., mean(EC)/mean(PM). The vehicle tests from each season are equally weighted, and averaged according to the calculated contribution to annual VMT in the Kansas City MSA (Table D-3). By using VMT and mass weighting, the profile scales up the contribution of older and higher emitting vehicles according to their high PM emissions, but also scales their down their contribution based on the relatively small number of vehicle miles traveled associated with these vehicles. For application in MOVES, the fleet-average profile is used to characterize $PM_{2.5}$ emissions across all model year groups, and all ages of vehicles used to represent deterioration.

Because the $PM_{2.5}$ speciation varied significantly by model year group,[48] the fleet average speciation profile is sensitive to the averaging assumptions. As mentioned above, we did not maintain the difference in speciation in model year groups, due to concern that the model-year groups would not be representative of the PM emissions as the vehicles aged. Given the uncertainty of the PM speciation profiles, we thought it would be unreasonable to model differences in PM speciation according to different ages of vehicle fleets in different areas in the US. For simplicity, we assume that the fleet-average $PM_{2.5}$ profile from Kansas City to be representative of the US gasoline fleet.

We recognize the need to incorporate speciation data on newer vehicles. For the next generation of vehicles, the composition of PM is expected to become increasingly dominated by black carbon emissions from both low-emitting port-fuel injected vehicles[49,55,56,57] and gasoline-direct injection (GDI) vehicles.[58,59,60] We plan on incorporating light-duty gasoline PM profiles to MOVES and SPECIATE as such data on representative, in-use vehicles become available.

The developed $PM_{2.5}$ profiles used in MOVES for gasoline exhaust are included in Table D-3. The number of samples for each $PM_{2.5}$ species are also shown in Table D-3. EC was measured on each vehicle test and has a much greater sample size than the other species. The EC and nonECPM emission rates in MOVES[41] are updated to be consistent with the EC fractions developed in Table D-3.

For application in MOVES, only the $PM_{2.5}$ species required by CMAQv5.1 are reported. A revision of the metal emission rates for Mn, Cr, and Ni for gasoline vehicles based on the KCVES is provided in the Fuels and Toxics Report. The $PM_{2.5}$ ratios that were not significantly greater than 0 at the 95 percent confidence intervals were reported as 0, which removed five $PM_{2.5}$ species pollutants from the start profile. Fuel samples analyzed for 171 of the vehicles tested in KCVES yielded an average fuel sulfur content of 161.2 ppm. Fuel sulfur content in the US is now lower after implementation of the Tier 2[61] and Tier 3[62] Gasoline Sulfur Standards (30 ppm beginning 2006-2008, and 10 ppm in 2017). In MOVES, the baseline sulfate emissions estimated from the $PM_{2.5}$ profile are adjusted according to the user-supplied fuel sulfur content as discussed in the fuel effects report.[39]

Details on the data, quality control measures, and statistical methods used to develop the profile are documented in the Sonntag *et al.* (2013).[48] The paper also introduces methods to identify significant measurements, correct for organic carbon positive artifact, control for contamination from the testing environment on the $PM_{2.5}$ speciation profiles, and impute missing $PM_{2.5}$ species in the KCVES measurements from other light-duty gasoline PM emission studies. Speciation factors for additional $PM_{2.5}$ species (P, Cu, Zn, Br, Mo, and Pb) that are not included in MOVES are also presented.

Table D-3 Gasoline $PM_{2.5}$ Profile for Start and Running Emissions Weighted Average using Vehicle Miles Traveled (VMT)

PM Species	Start (8992)			Running (8993)		
	n	mean ratio +/- 95% CI		n	mean ratio +/- 95% CI	
Elemental Carbon (EC)	484	44.37%	+/- 4.30%	531	14.00%	+/- 2.68%
Organic Carbon (OC)	66	42.64%	+/- 6.63%	99	55.70%	+/- 4.02%
Non-carbon Organic Matter (NCOM)	66	8.53%	+/- 1.33%	99	11.14%	+/- 0.80%
SO4	66	0.95%	+/- 0.24%	99	7.19%	+/- 1.90%
NO3	66	0.26%	+/- 0.08%	99	0.29%	+/- 0.08%
NH4	66	0.43%	+/- 0.10%	99	2.78%	+/- 0.73%
Fe	66	0.31%	+/- 0.21%	99	1.83%	+/- 0.53%
Al				99	0.32%	+/- 0.10%
Si				99	0.32%	+/- 0.10%
Ti				99	0.03%	+/- 0.01%
Ca	66	0.39%	+/- 0.14%	99	1.44%	+/- 0.26%
Mg	66	0.02%	+/- 0.02%	99	0.14%	+/- 0.02%
K				99	0.09%	+/- 0.03%
Mn				99	0.02%	+/- 0.02%
Na	66	0.01%	+/- 0.00%	99	0.04%	+/- 0.01%
Cl	66	0.02%	+/- 0.01%	98	0.10%	+/- 0.04%
Unspeciated (PMOTHR)	66	2.09%	+/- 1.75%	99	4.56%	+/- 1.10%

D.2 Development of E55/59 Profile for Use in MOVES2014 for Pre-2007 Conventional Diesel

An updated $PM_{2.5}$ profile for pre-2007 conventional diesel trucks was developed from the CRC E55/59 Study: Heavy-Duty Vehicle Chassis Dyno Testing for Emissions Inventory.[63] The E55/59 program is the current source for $PM_{2.5}$ emission rates for medium- and heavy-duty conventional diesel trucks in MOVES, and is the source of the conventional diesel TOG speciation profiles. By using the E55/59 study for $PM_{2.5}$ speciation profiles, we are using a consistent study with both the $PM_{2.5}$ emission rates and the TOG speciation profiles in MOVES.

The E55/59 $PM_{2.5}$ profile includes measurements from eight heavy-duty trucks, ranging from a 1985 to 2004 model year as shown in Table D-4..The E55/59 average sulfur content is 172 ppm. The CRC E55/59 study was conducted from 2001-2005 in several phases. Chemical characterization of $PM_{2.5}$ emissions was conducted for nine of the 75 trucks tested in the E55/59 study, ranging from 1985 to 2004 model year.

Table D-4 Vehicle Information from the Speciated E55/59 Trucks

Phase	ID	Medium/Heavy-Duty	Vehicle Model Year	Vehicle Manufacturer	Engine Model Year	Engine Model	Engine Power (hp)	Engine Disp. (Liter)	Engine Manufacturer	Odometer Reading (mi)
1	1	H	1994	Freightliner	1994	Series 60	470	12.7	Detroit	639105
1	2	H	1995	Freightliner	1995	3406B	375	14.6	Caterpillar	241843
1	3	H	1985	International	1985	NTCC-300	300	14	Cummins	501586
2	39	H	2004	Volvo	2003	ISX	530	14.9	Cummins	45
2	40	H	2004	Freightliner	2003	Series 60	500	14	Detroit	8916
2	41	M	1998	Ford	1997	B5.9	210	5.9	Cummins	13029
2	42	H	2000	Freightliner	1999	3406	435	14.6	Caterpillar	576998
2	43	H	1995	Peterbilt	1994	Series 60	470	12.7	Detroit	899582
2	44	H	1989	Volvo	1989	3406	300 (est.)	14.6	Caterpillar	811202

In all, 65 tests were conducted on the nine trucks selected for PM speciation. Phase 1 tested three heavy heavy-duty diesel trucks (HHDDTs) for PM speciation on four modes of the Urban Dynamometer Driving Schedule (UDDS), including: idle, creep, transient and cruise. Phase 2 tested six additional heavy heavy-duty diesel trucks, and one medium heavy-duty diesel truck (MHDDT). In Phase 2, the HHDDTs were also tested on the UDDS, as well as a high-speed cruise mode added after Phase 1. The MHDDT was tested on MHDDT schedule developed by the California Air Resources Board that included two transient modes and a cruise mode. For chemical speciation, some tests were repeated in sequence to collect additional mass on the filter, including extended idle and extended creep. In Phase 2, the speciation data was not collected for the creep mode.[63]

The total and speciated $PM_{2.5}$ emissions data from the E55/59 study was compiled from the speciation database compiled in CRC Report No. E75-2: Diesel Unregulated Emission Characterization Report[64] and from Table 17 of the E55/59 Phase 1 report.[65] The data reduction steps used to develop a $PM_{2.5}$ speciation profile from the E55/59 speciated data are outlined in the following Steps: 1-4.

Step 1. We first calculated the average $PM_{2.5}$ profile for each individual truck and four generic classifications of test cycle, namely: idle, creep, cruise, and transient. The composite UDDS cycle is classified as a transient cycle, similar to the classification conducted of speciation profiles by E75-2.[63] The truck and test cycle average PM profiles are calculated as ratios of the means, also called a PM mass-weighted profile. In this manner, idle tests that contain three repeat idle cycles contribute more to the average than tests that include only one idle cycle. The average profile for each vehicle/test cycle classification is shown in Figure D-1. Thirty average speciation profiles were calculated from the 65 tests as shown in Figure D-1. Typically, each truck/cycle average contains two tests.

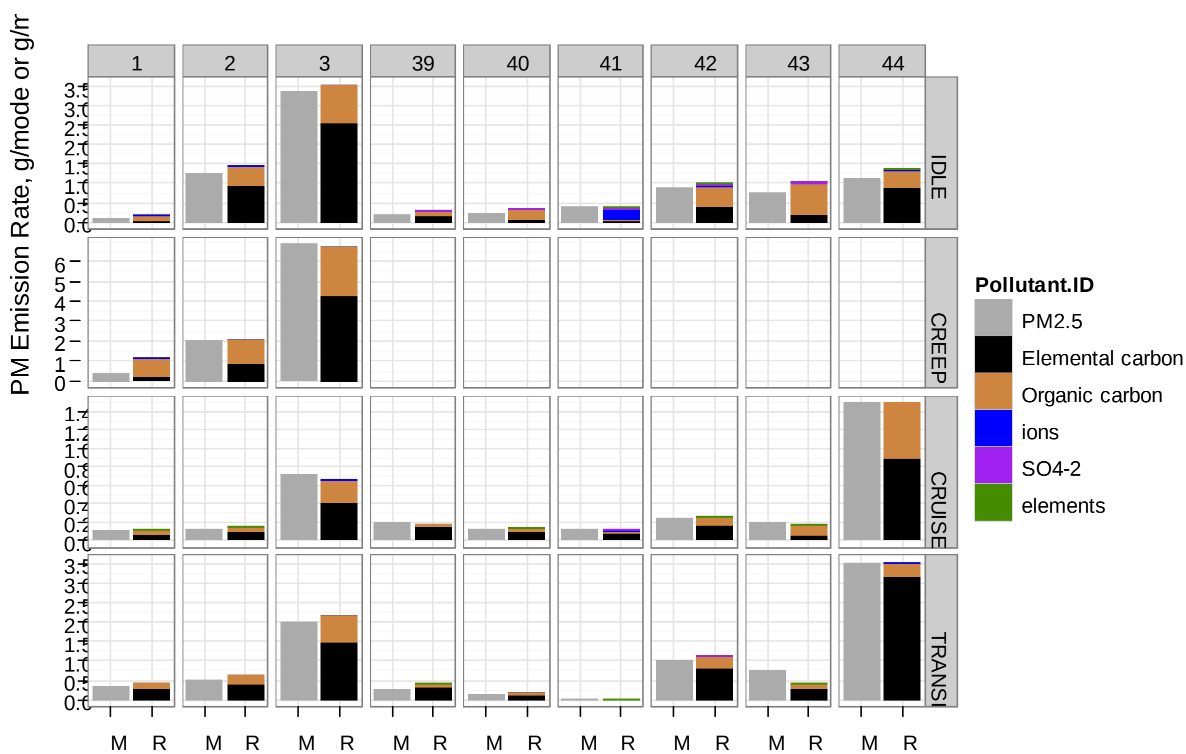

Figure D-1 Average $PM_{2.5}$ Speciation Profiles by Truck and Test Cycle from the E55/59 Program. M = Measured total $PM_{2.5}$, R = Reconstructed Total $PM_{2.5}$ from the Speciated Measurements

Step 2. We removed the average $PM_{2.5}$ profiles with suspect data. As shown in Figure D-1, the MMHDT truck (Truck 41) had very low PM emissions on the transient cycle, and a very large contribution of ammonium to the idle cycle. This PM composition does not compare well with previous data in the literature[66], so the medium-duty truck was removed from further analysis.

Step 3. We calculated a median PM profile using the individual truck/test-cycle PM profiles calculated in steps 1 and 2. The median is used rather than the mean due to the small sample (eight trucks), in contrast to the variety of truck technologies, exhaust control systems, and ages of the trucks in the real-world fleet. A mass-weighted mean would have been dominated by the results for Truck 3 and Truck 44, which had the highest PM emission rates. Instead we calculated the median of the PM fractions, and not a fraction of the median emission rates. In this manner, the final PM speciation profile is not overly dependent on any one vehicle. Additionally, there may be systematic differences between the Phase 1 and Phase 2 measurements that could impact a mass-weighted profile. By calculating the $PM_{2.5}$ species fraction before computing the median, any differences impacted the absolute $PM_{2.5}$ emission rates between phases do not impact the resulting speciation profile.

Step 4. We adjust the median profile to account for unmeasured $PM_{2.5}$ species including metal-bound oxygen and non-carbon organic matter. The additional oxygen mass associated with the metal oxides are calculated using the oxide state assumptions in Sonntag *et al.* (2013)[48] reproduced in Table D-5.

Table D-5 Oxide States Assumed for Calculation of Metal-Bound Oxygen

Element	Oxide Form 1	Oxide Form 2	Oxide Form 3	Oxide/Element Mass Ratio
Na	Na_2O			1.35
Mg	Mg			1.0
Al	Al_2O_3			1.89
Si	SiO_2			2.14
P	PO_4			3.07
Cl	Cl			1.0
K	K_2O			1.20
Ca	Ca			1.0
Ti	TiO_2			1.67
Cr	Cr_2O_3	CrO_3		1.69
Mn	MnO	MnO_2	Mn_2O_7	1.63
Fe	FeO	Fe_2O_3		1.36
Ni	NiO			1.27
Cu	CuO			1.25
Zn	Zn			1.0
Rb	Rb_2O			1.09
Br	Br			1.0
Mo	MoO_2	MoO_3		1.42
Pb	PbO	PbO_2		1.12

For the Phase 1 samples, the molar concentration of ammonium balances within 5 percent of the molar concentrations of $2*SO_4 + NO_3$. This is what would be expected if the ammonium exists as ammonium sulfate $[NH_4]_2SO_4$ and ammonium nitrate, NH_4NO_3. For the Phase 2 samples, ammonium balances within 25 percent of the molar concentrations of $2*SO_4 + NO_3$. Due to the relatively good agreement between the measurements, it appears that the sulfate on the filter exists as ammonium sulfate. As such, we did not account for sulfate-bound water contributing to filter mass.

The sum of the PM fractions from the median profiles is greater than one. To achieve mass balance, we are scaled down the organic carbon fraction to correct for positive artifact inherent in organic carbon (OC) filter measurements, as was done in previous work including for the light-duty gasoline profile[48] and analysis of emissions from other combustion sources.[67] We calculated the organic matter (OM) as the remainder of the $PM_{2.5}$ using Equation 11.

$$OM\% = 100 - EC\% - elements\% - metal\ bound\ oxygen\% - ions\% \quad \textbf{Equation 11}$$

Then, we split the OM into OC and non-carbon organic matter (NCOM) using the following relationship: OM = 1.2 * OC used by Kleeman *et al.* (2000)[68] and developed from work conducted on medium-duty diesel emissions[66], as shown in Equation 12 and Equation 13.

$$OC\% = \left(\frac{5}{6}\right) OM\% \quad \textbf{Equation 12}$$

$$NCOM\% = \left(\frac{1}{6}\right) OM\% \quad \textbf{Equation 13}$$

The initial and corrected OC/PM factors are shown in Table D-6. The adjusted OC speciation factors are smaller than the initially measured OC/PM fraction, which is expected due to the higher affinity for OC artifact to collect on the quartz fiber filters, as compared to the Teflon filters used to measure $PM_{2.5}$ mass.[69]

Table D-6 Impact of Mass-Balance Correction on Organic Carbon and Organic Matter Emission Rates

PM factors	IDLE	CRUISE	TRANSIENT
Initial OC/PM factor	54.1%	36.3%	30.1%
Mass-balance OM/PM factor	41.7%	36.1%	17.4%
Corrected OC/PM factor	34.7%	30.1%	14.5%

The resulting profiles for the $PM_{2.5}$ species are located in Table D-7. The Start/Extended Idle profile is based on the idle test cycles, and the running emissions are based on the transient cycles. These cycles are selected for use for modeling these emission processes because they have similar PM characteristics (EC/PM) ratio as the $PM_{2.5}$ MOVES emission rates for conventional diesel as discussed next.

Table D-7 $PM_{2.5}$ Profiles for Conventional Diesel Exhaust Developed for MOVES2014

	Idle (Profile 8994)	Running (Profile 8995)
Elemental Carbon	46.40%	78.97%
Organic Carbon	34.74%	14.52%
NonCarbon OM	6.95%	2.90%
SO4	5.27%	1.03%
NO3	1.25%	0.18%
NH4	1.74%	0.36%
Fe	0.34%	0.13%
Al	0.06%	0.06%
Si	0.30%	0.22%
Ti	0.01%	0.01%
Ca	0.58%	0.35%
Mg	0.13%	0.01%
K	0.26%	0.02%
Na	0.31%	0.03%
Cl	0.38%	0.13%
CMAQ5.0 unspeciated	1.28%	1.09%

In MOVES, the EC/PM fraction from the Idle profile (8994) is used for idle emissions from running (opModeID 1, processID 1) and extended idle (processID 90). It is also used to speciate the PM from start emissions (processID 2) and auxiliary power emissions (processID 91). The running profile is used to speciate the PM from all other operating modes from running emissions (processID 1). For typical MOVES county-runs, running emissions contribute over 80 percent of the $PM_{2.5}$ emissions from conventional diesel trucks.

The MOVES conventional diesel profiles developed from the E-55/59 Study are compared to composite profile developed by Schauer *et al.* (2006)[54] from measurements taken from the DOE Gasoline/Diesel PM Split Study, from Shah et al. (2004)[70] from measurements made at CE-CERT, and the NFRAQS heavy-duty diesel profile (SPECIATE Profile 91106) in Table D-8. The EC/PM fraction from the E55/59 transient cycle compares well to both the composite profiles. The E55/59 idle profile has a substantially lower EC/PM fraction than the composite profiles, with a corresponding higher fraction of organic matter. The cold/start idle profile from Shah et al. (2004) also shows an even lower EC/PM fraction during idle than high load conditions, with a substantially lower EC/PM fraction. The MOVES sulfate fractions appear to be more aligned with the DOE Split study, which could be due to newer technology diesel and lower altitude testing. Elements and ion emission rates compare well to the DOE gasoline/diesel PM split study.

Table D-8 Comparison of MOVES Conventional Diesel Profiles with other $PM_{2.5}$ Conventional Diesel Profiles

	MOVES E-55/59		CE-CERT 2004[a]		DOE Gasoline/ Diesel PM Split Study	Northern Front Range Air Quality Study
	Idle (8994)	Running (8995)	Cold start/Idle	Running (Transient)	Composite	Composite (91106)
Elemental carbon	46.4%	79.0%	13.3%	68.0%	72.7%	77.1%
Organic matter	41.7%	17.4%	81.4%	33.5%	24.1%	17.6%
SO_4-2	5.3%	1.0%			1.3%	0.3%
Cl + NH_4 + NO_3	3.4%	0.7%			0.4%	0.1%
Elements	2.1%	1.1%			1.5%	0.5%

Note:
a. Organic matter estimated using the 1.2 * OC, other components not measured.

D.3 Development of the ACES PM2.5 Profile for 2007 and Newer Technology Diesel

The $PM_{2.5}$ speciation profile for 2007-and-later technology is based on Phase 1 of the Advanced Collaborative Emissions Study (ACES) Report.[20] The purpose of the ACES report was to characterize criteria and toxic emissions from advanced technology diesel engines and control systems. Phase 1 of ACES tested four heavy-duty diesel engines each equipped with a catalyzed diesel particulate filter (C-DPF). The $PM_{2.5}$ profile is based on a 16-hour cycle which is composed of FTP and CARB 5-Modes, developed specifically to gain sufficient PM mass to measure the emission rates of trace metals and toxics and to capture diesel particulate filter regeneration events. The $PM_{2.5}$ measurements from the 16-hour cycle include the exhaust measurements downstream of the C-DPF and crankcase blow-by emissions. Crankcase blow-by emissions contributed 38 percent of the combined crankcase and tailpipe $PM_{2.5}$ emissions on the FTP cycle.

The SPECIATE contractor (Abt Associates) developed the $PM_{2.5}$ profile from the ACES program Phase 1 with input from the US EPA, with the intent of maintaining consistency with the summarized results in the ACES Phase 1 report. The 16-hour results yielded the most accurate measurements at the low levels of $PM_{2.5}$ and are used to represent all $PM_{2.5}$ emission processes from 2007-and-newer on-highway diesel vehicles.

The following decisions were made to develop a profile to be consistent with the results in the ACES Phase 1 report.

1. The original measurements were used rather than background or tunnel corrected measurements. EC and OC were not corrected for background, or backup quartz filters. Background correcting the EC/OC filters caused negative EC/OC emission rates on three of the four engines. The ACES researchers did not report OC corrected by a backup-quartz filter because of concern of under-representing OC emissions.[71]

Similarly, species for elements and ions were not corrected for tunnel blanks. Using uncorrected OC measurements likely contributed to the mass of the sum of the speciated measurements being higher than Teflon filter measurements.[72] By using the original measurements, rather than the background or tunnel corrected measures, we are likely overestimating the emissions from some of the individual species that are subject to positive artifact like OC. The ACES researchers discuss possible approaches for correcting the measured OC emission rates, and mention this as an area for future work for 2007 diesel engines.

2. Unmeasured species that likely contribute to particulate matter were not included in the profile, including sulfate-bound water and metal-bound oxygen from the profile. The PM collected on the filter were analyzed for nitrate and ammonium, however no ammonium or nitrate was detected.[20] In the absence of these species, the sulfate is expected to exist as hydrated sulfuric acid. Khalek *et al.* 2011[71] reported that accounting for the water-bound sulfate would increase the summed mass of the individual species 37 percent beyond the measured filter mass. Rather than lowering the factors for other species by including the sulfate-bound water, it was excluded from the profile. Converting the measured organic carbon to organic matter and accounting for the oxide state of the elements was considered by Khalek *et al.* (2011)[71], but was not conducted due to the uncertainty of reconciling the filter mass and the sum of the measured species.

3. According to the SPECIATE database, the profile was normalized to the gravimetric mass of PM. Gaseous and particulate phase sulfate are combined in the PM profile. More information on the profile itself can be found in the SPECIATE database, and the database's supporting documentation outlines specific procedures for creating PM profiles.[73]

The ACES Profile is included in the SPECIATE database as profile #5680. This profile is the basis of SPECIATE profile 8996 used in MOVES with one adjustment. MOVES needs organic matter reported as OC and non-carbon organic matter (NCOM). We treated the reported OC in the SPECIATE profile 5680 as OM, and calculate OC and NCOM using the same split (Equation 12) as used for conventional diesel and light-duty gasoline. The species not needed by MOVES from the ACES Phase 1 profile are summed into the Unspeciated fraction. The speciation values are presented in Table D-9. Metal emission rates for manganese, chromium, and nickel from MOVES are derived from the ACES Phase 1 data.[4] They are estimated using the metals calculator with mass/distance emission rates, and are not reported in the SPECIATE profiles.

Table D-9 SPECIATE $PM_{2.5}$ Profile 8996 Developed from the 16-hour Cycle from Four Heavy-duty Diesel Engines with Catalyzed-DPFs in the ACES Phase 1 Program

	Weight %
Elemental Carbon	9.98%
Organic Carbon	22.33%
Non Carbon Organic Matter	4.47%
Sulfate	59.91%
Nitrate	0.00%
Ammonium	0.00%
Iron	0.64%
Aluminum	0.11%
Silicon	0.09%
Titanium	0.02%
Calcium	0.47%
Magnesium	0.14%
Potassium	0.05%
Sodium	0.99%
Chlorine	0.04%
Unspeciated	0.78%

The 2007+ diesel EC/PM fraction in MOVES is a constant 8.61 percent based on previous analysis documented in the heavy-duty diesel report. This value is quite similar to the 9.98 percent EC/PM fraction estimated from Phase 1 of the ACES program. Due to the similarity in the EC/PM fraction, the previous value of 8.61 percent is also used in MOVES. However, the ACES Phase 1 data is used to speciate the remaining species listed in.

D.4 Development of the Compressed Natural Gas (CNG) Profile

The California Air Resource Board (CARB) conducted several emission characterization studies on compressed natural gas vehicles. We used test data collected on CNG New Flyer bus with a 2000 MY Detroit Diesel (DDC) Series 50G engine, equipped with and without an oxidation catalyst to develop $PM_{2.5}$ speciation profiles. CARB also conducted tests on a CNG bus with a 2001 Cummins Westport engine. We developed the profile on the DDC engine, with and without catalyst to estimate the impact of oxidation catalyst control, without introducing differences in engine technology. CARB characterized the PM emissions on a steady-state cycle, and a central business district cycle (CBD). We used the CBD data, which was consistent with the criteria pollutant analysis in the MOVES201X Heavy-duty Emissions Report and was considered more representative of typical transit bus behavior.

We elected to use only the data reported by CARB on the DDC 50G engine to develop the profile. Using a single profile provides consistency in the PM characterization estimates and assures that the organic carbon emissions are reduced with implementation of oxidation catalyst controls. Other studies that reported EC/OC did not measure emission rates for elements.[74] We used measurements made on the same tests to construct the profile in Table D-10. The PAH/OC ratios documented in the MOVES201X toxics report[4] were also developed from the CARB measurements on the DDC 50G.

Table D-10 $PM_{2.5}$ Speciation Profiles for CNG Compressed Ignition Transit Bus Exhaust

Pollutant	Uncontrolled (95219)	Oxidation Catalyst (95220)
Elemental Carbon (EC)	9.25%	11.12%
Organic Carbon (OC)	36.99%	37.45%
Non-carbon Organic Matter (NCOM)	7.40%	7.49%
SO4	0.64%	1.04%
aluminum	0.89%	0.89%
calcium	0.21%	0.44%
chromium	0.25%	0.25%
cobalt	0.39%	0.40%
iron	0.25%	0.25%
nickel	0.04%	0.00%
phosphorus	0.04%	0.15%
silicon	0.46%	0.59%
zinc	0.14%	0.20%
Unspeciated $PM_{2.5}$	43.04%	39.74%

We used PM, EC, OC, and element emission rates for two repeat tests both with and without the oxidation catalyst.[75,76] CARB measured 13 elements by X-ray fluorescence but no ions (sulfate, ammonium, or nitrate) were measured. The sulfate emissions were estimated by assuming that all elemental sulfur is in the form of sulfate. This assumption is consistent with sulfate and elemental sulfur measurements reported for natural gas combustion in the speciate database (SPECIATE 91112). We assume that the missing ammonium and nitrate emissions are zero, based on the negligible ammonium and nitrate measurements from modern spark-ignition CNG buses equipped with three-way catalysts.[77] Sodium and magnesium were the largest elements measured (sodium was over 7 percent of the $PM_{2.5}$ measured in the uncontrolled test), which is likely due to known measurement artifact for XRF measurements of sodium and magnesium. As such the sodium and magnesium emission rates are reported as zero.

The use of the oxidation catalyst reduced the $PM_{2.5}$ emission rates from 28 mg/mile to 20.3 mg/mile on the CBD cycle (a 27.5 percent decrease). As shown in , the composition of the $PM_{2.5}$ stayed fairly constant. The EC and OC fractions between the two control conditions are not statistically different. The estimated sulfate emissions are significantly higher with the oxidation catalyst, which is to be expected. Both profiles contain a large amount of unspeciated $PM_{2.5}$ emissions. The source of the large unspeciated $PM_{2.5}$ emissions is unknown, but may be attributed to the different sampling media for the total and speciated $PM_{2.5}$ emissions, which is amplified at the low $PM_{2.5}$ concentrations measured from CNG exhaust. The absence of ion measurements may also be a contributing factor.

The real-world variability in the $PM_{2.5}$ composition is larger than the developed profiles suggest. The OC/PM fraction for the 2001 Cummins Westport with oxidation catalyst was 61.9 percent, which is much larger than that measured on the 2000 Detroit diesel engine. Lanni *et al.* (2003)[74] reported that the OC/PM fraction on three CNG transit buses with DDC Series 50G engines ranged from 29 percent to 74 percent of the $PM_{2.5}$. The EC emissions measured by Lanni *et al.* (2003)[74] were below the detection limit, but the presented results compare well with the 2001 Cummins Westport measured by CARB (12.7 percent EC/PM). The sulfate fraction for the oxidation catalyst presented in compares well with the sulfate fraction reported for the 2001 Cummins Westport by CARB[76] (2.8 percent), and by Lanni *et al.* (2003)[74] (1.5 percent to 2.4 percent).

Appendix E PM$_{10}$/PM$_{2.5}$ Factors

The gasoline PM$_{10}$/PM$_{2.5}$ factor is based on measurements of 1991-1997 model year vehicles tested by Norbeck *et al.* (1998).[78] This ratio estimates that roughly 10 percent of the PM emitted from gasoline vehicles is in the coarse range, which agrees with the size-distributions reported from cascade impactor measurements on light-duty gasoline exhaust from Schauer *et al.* (2008).[79]

The diesel PM$_{10}$/PM$_{2.5}$ factor is based on a 1985 EPA report[80], which reports that 92 percent of particulate mass is measured below a 2.5 µm cut-off. Although derived from measurements on older technologies, the diesel PM$_{10}$/PM$_{2.5}$ ratio compares well with observations of the particle size distribution of diesel exhaust by Kittelson *et al.* (1998)[81], who states that the coarse mode contains 5-20 percent of the total aerosol mass. Unfiltered crankcase emissions published by Donaldson Company Inc. (2011)[82] have similar reported mass distributions with ~ 93 to 97 percent of the cumulative mass particles smaller than 2.5 µm. In contrast, Tatli and Clark (2008)[83] report that the particle mass size distribution is significantly different from crankcase and tailpipe diesel emissions for particles below 1 µm. Due to the limited information on coarse-mode crankcase particulate emissions, we assume the same PM$_{10}$/PM$_{2.5}$ fraction for diesel crankcase emissions.

Filtered diesel crankcase and exhaust emissions are expected to have smaller PM$_{10}$/PM$_{2.5}$ ratios, due to the higher filter capture efficiency of coarse mode particles.[82,84] However, the same PM$_{10}$/PM$_{2.5}$ ratios are used for the later model year groups, due to limited coarse mode particulate exhaust measurements, and limited information on the failure rates of these technologies in real-world use.

No information was available on the PM$_{10}$/PM$_{2.5}$ ratios for CNG emissions, and the gasoline ratio is used for CNG emissions. Table E-1 contains the selected exhaust PM$_{10}$/PM$_{2.5}$ ratios used in MOVES.

Table E-1 PM$_{10}$/PM$_{2.5}$ Ratios for Primary Exhaust and Crankcase Emissions by Fuel Type

Fuel	PM$_{10}$/PM$_{2.5}$
Gasoline, E85, CNG	1.130
Diesel	1.087

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