MOVES

Motor Vehicle Emission Simulator

Updates to Total Organic Gases (TOG) Calculations in MOVES

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Total Organic Gases in MOVES

- TOG = hydrocarbons plus oxygenated hydrocarbons (e.g. aldehydes, alcohols)

- MOVES2014 used Total Hydrocarbon (THC) emission rates to estimate all other organic gas aggregates (NMHC, VOC, NMOG, TOG) through a series of calculations

NMHC: Non-Methane Hydrocarbons
NMOG: Non-Methane Organic Gases
VOC: Volatile Organic Compounds
CH_4: Methane

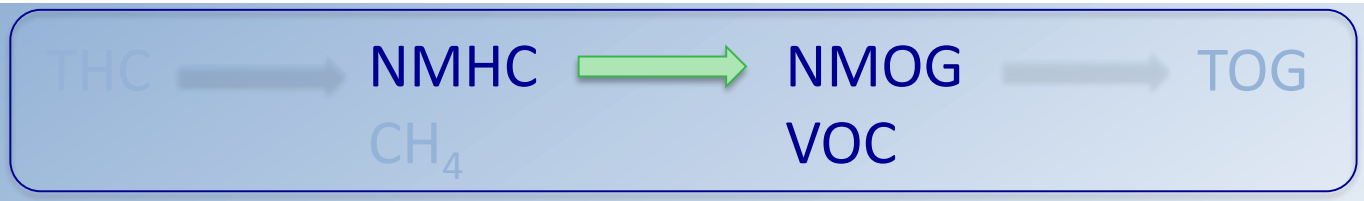
Calculating CH_4 and NMHC

- In MOVES, methane is calculated as a fraction of THC

$$NMHC = THC \times \left[1 - \frac{CH_4}{THC}\right]$$

$$CH_4 = THC \times \frac{CH_4}{THC}$$

Calculating NMOG and VOC



- In MOVES 2014, NMOG and VOC are calculated using conversion factors referred to as ***speciationConstant***

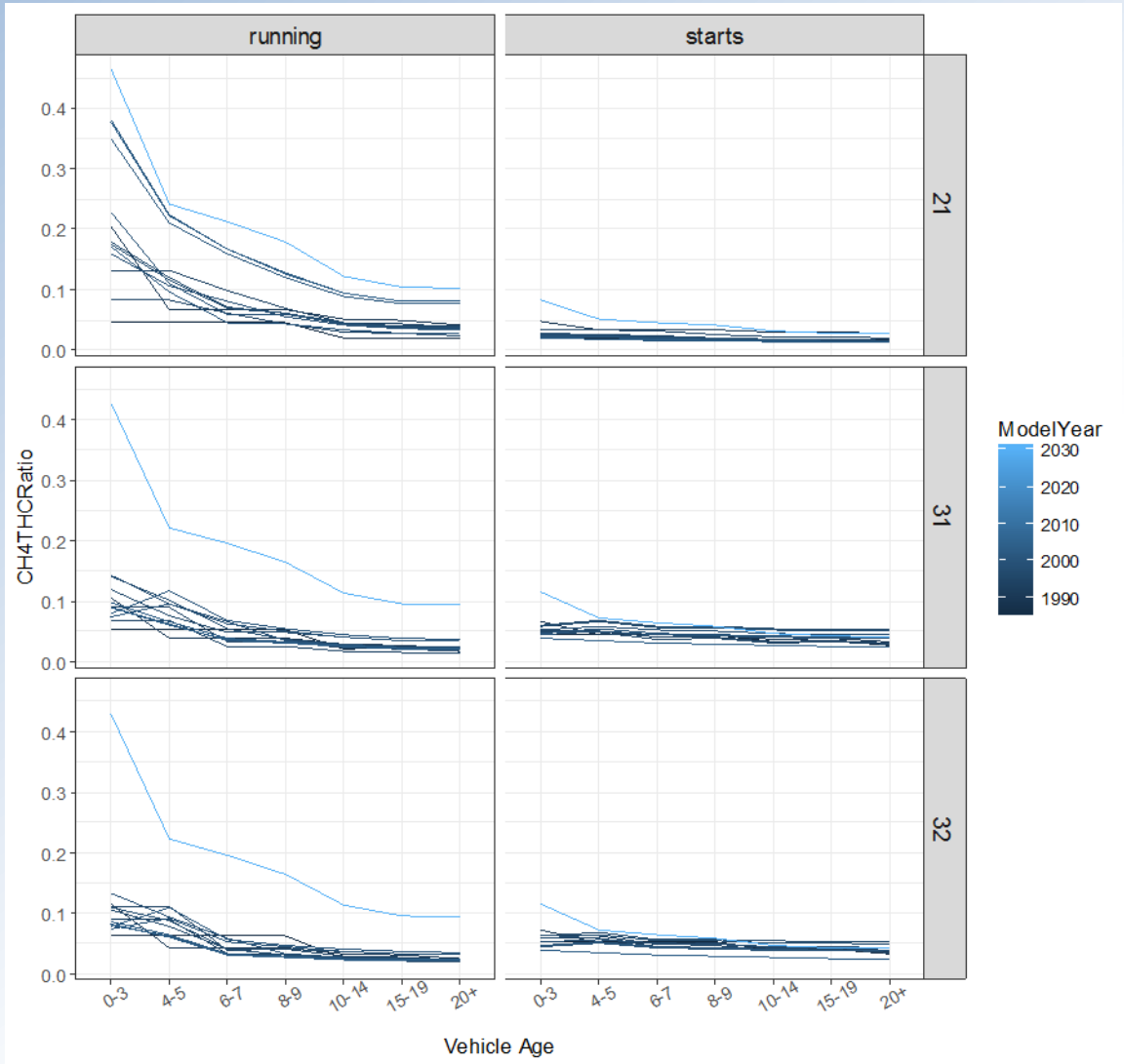
$$NMOG = NMHC \times \frac{NMOG}{NMHC} + \sum_{i=1}^{4}(A_i \times B_i \times C_i)$$

$$VOC = NMHC \times \frac{VOC}{NMHC} + \sum_{i=1}^{4}(A_i \times B_i \times C_i)$$

Where:
A = oxySpeciation
B = oxyMassFraction
C = oxyVolume
i = gasoline oxygenates (ethanol, MTBE, ETBE, TAME)

Motivation for updating CH_4/THC

- CH_4/THC ratios in MOVES2014 are based on a CH_4 emission rate for running and a CH_4 rate for starts
  - Based on emission test results[1]
- Data available for THC emission rates varied with opModes and age among other factors
- Data for CH_4 emission rates did not vary with opModes or age, resulting in decreases in CH_4/THC ratios with age
- For next public release, we want a simpler, more transparent derivation of CH_4/THC ratios consistent with other TOG calculations



Note: Plot only shows LD for illustrative purposes but the age trend applies to all sourcetypes

[1] From FTP emission results and other supplemental information as described in EPA-420-R-15-003

Proposed updates to CH_4/THC: Data

- For the next MOVES release, we suggest to calculate CH_4/THC ratios based on each SPECIATE* profile used in MOVES
  - SPECIATE profiles used in MOVES cover all sourcetypes and processes
  - Further detail on specific code changes provided in the appendix
- For Tier 2 vehicles running on low-level ethanol blends, we propose to include CH_4/THC ratios for cold-starts and running emissions based on bag-specific data from EPAct Phase I
- For CNG exhaust, we are considering the use of ARB measurements not currently included in the SPECIATE database

*SPECIATE: online EPA speciation database https://cfpub.epa.gov/speciate/

Proposed updates to speciationConstant parameters

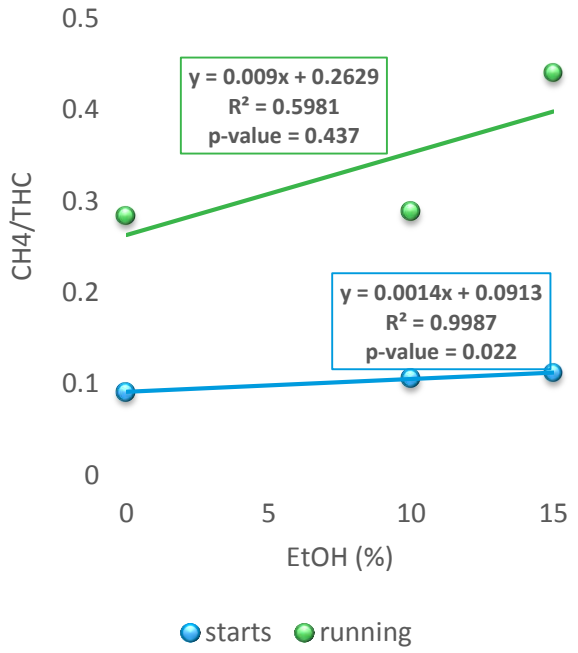
- For the next MOVES release, we suggest calculating NMOG/NMHC and VOC/NMHC ratios based on each SPECIATE profile used in MOVES

- For Tier 2 vehicles running on low-level ethanol blends, we propose to include NMOG/NMHC and VOC/NMHC ratios for cold-starts and running emissions based on bag-specific data from EPAct Phase I

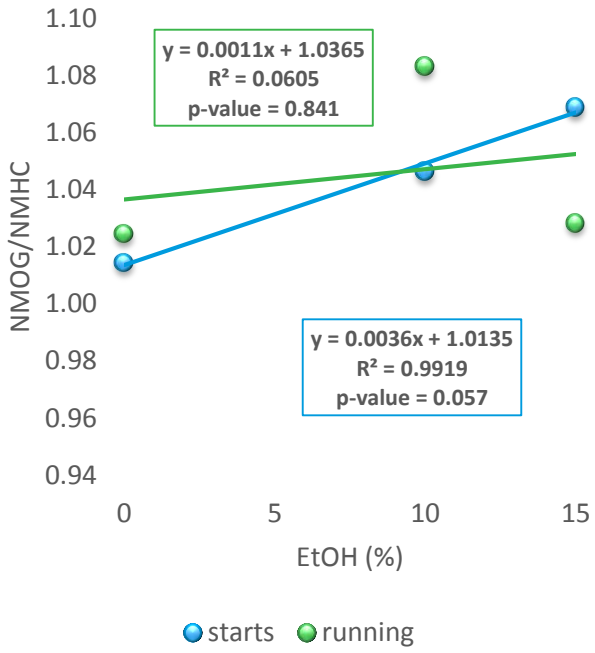
Analysis of EPAct Phase I data for Tier 2 vehicles

- Each point corresponds to the ratio of means for all tests considered at each ethanol level:

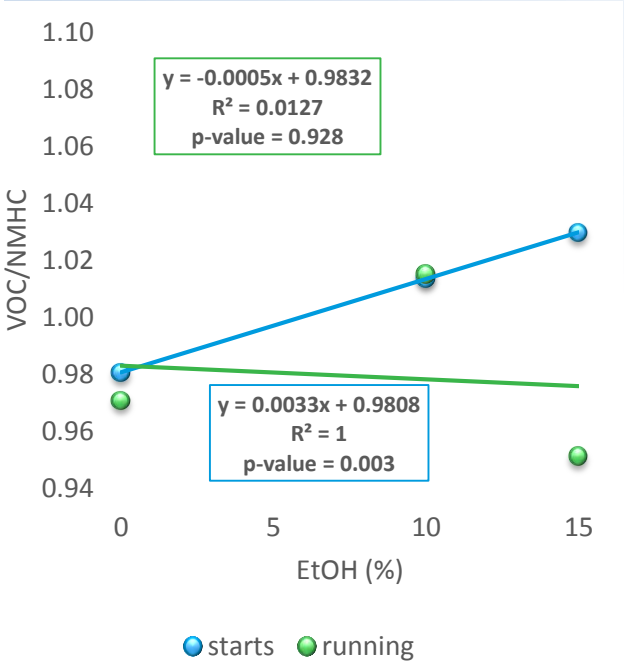
CH_4/THC



NMOG/NMHC



VOC/NMHC



- The linear fit model suggests that the relationship with ethanol composition is statistically significant for starts but not for running emissions

Analysis of EPAct Phase I data for Tier 2 vehicles (cont'd)

- For Tier 2 vehicles, we propose the use of CH_4/THC, NMOG/NMHC and VOC/NMHC that vary with ethanol levels (0-15%) for starts while using a constant ratio for the running emission process.

Ethanol (%)	CH_4/THC		NMOG/NMHC		VOC/NMHC	
	starts	running	starts	running	starts	running
0	0.091	0.338	1.014	1.038	0.981	0.974
5	0.098	0.338	1.031	1.038	0.997	0.974
8	0.102	0.338	1.042	1.038	1.007	0.974
10	0.105	0.338	1.046	1.038	1.014	0.974
15	0.112	0.338	1.069	1.038	1.030	0.974

*A table relating the new proposed ratios with MOVES parameters and SPECIATE profiles is presented in the appendix.

Implications to NMOG and VOC calculations

- New methodology does not allow the determination of parameters used to correct for oxygenated volume of fuel.
- However, these adjustments have become less relevant as MTBE, ETBE and TAME are removed from the market, supporting the idea of eliminating these adjustments from the algorithm.

$$NMOG = NMHC \times \frac{NMOG}{NMHC} + \sum_{i=1}^{4} (A_i \times B_i \times C_i)$$

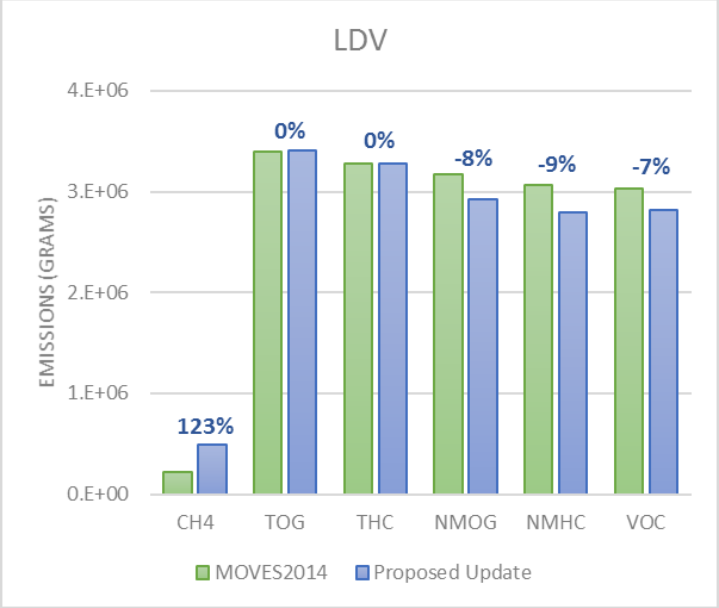
$$VOC = NMHC \times \frac{VOC}{NMHC} + \sum_{i=1}^{4} (A_i \times B_i \times C_i)$$

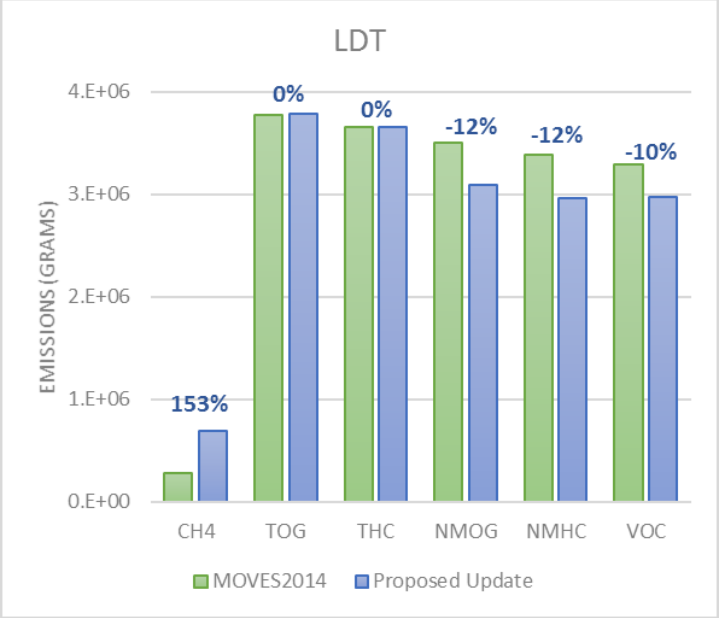
- MOVES includes profiles for fuel subtypes E0, E5, E8, etc. Thus, ethanol impacts could still be included.

Impact on the Inventory*

- Case Study:
  - New Mexico, July 2015
  - LDV, LDT only
  - Fuel sales set to 100% E10
  - Modified CH_4/THC and speciationConstants for Tier 2 vehicles running on E10
  - Results shown for MY >2000
- Large increase in CH_4 emissions
  - For New Mexico, this would represent increasing CH_4 share of GHG emissions from 0.005% to 0.015% for the onroad non-diesel light-duty sector (2014 NEI)
- Overall, changes result in a decrease in emissions of NMOG, NMHC and VOC of ~10%
- TOG change is negligible (TOG = NMOG + CH_4). Decrease in NMOG is offset by increase in CH_4

*A full assessment will be performed when the new code is delivered.





Summary

- For the next MOVES release, we propose to update CH_4/THC ratio to be consistent with other TOG calculations and data
- We propose to remove the age effect which is expected to significantly increase the methane from gasoline vehicles
- Overall, it is expected that updates in speciationConstant parameters will result in negligible changes of TOG emissions

APPENDIX

CH_4/THC and speciationConstant parameters for SPECIATE profiles

Profile number	Profile description	Emission Process	Fuel Subtype	Affected vehicles	CH_4/THC	NMOG/NMHC	VOC/NMHC
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 gas All MC and non-LD gas	0.142	1.024	0.996
8751a	Pre-Tier 2 E10 exhaust	Running, starts exhaust and crankcase.	RFG, E10, E8, E5	Pre-2001 LD gas All MC and non-LD gas	0.146	1.037	1.008
8753	E0 Evap	Evaporative (vapors, leaks), refueling spillage	Conventional Gasoline	All gas	0	1	1
8754	E10 Evap	Evaporative (vapors, leaks), refueling spillage	E10, E8, E5	All gas	0	1.071	1.071
8766	E0 Evap perm	Evaporative Permeation	Conventional Gasoline	All gas	0	1	1
8769	E10 Evap perm	Evaporative Permeation	E10, E8, E5	All gas	0	1.129	1.129
8770	E15 Evap perm	Evaporative Permeation	E15, E20	All gas	0	1.175	1.175
8774	Pre-2007 MY HDD exhaust	Running, starts, extended idle exhaust and crankcase. APU Running, starts exhaust and crankcase.	Diesel, biodiesel	Pre-2007 diesel Pre-2024 APU Pre-2007 LD diesel	0	1.145	1.124

CH_4/THC and speciationConstant parameters for SPECIATE profiles (cont'd)

Profile number	Profile description	Emission Process	Fuel Subtype	Affected vehicles	CH_4/THC	NMOG/NMHC	VOC/NMHC
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			
95335	2011+ 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			
8869	E0 Headspace	Refueling displacement vapor loss	Conventional Gasoline	All gas	0	1	1
8870	E10 Headspace	Refueling displacement vapor loss	E10, E8, E5	All gas	0	1	1
8871	E15 Headspace	Refueling displacement vapor loss	E15, E20	All gas	0	1	1
8872	E15 Evap	Evaporative (vapors, leaks), refueling spillage	E15, E20	All gas	0	1.118	1.118
8934	E85 Evap	Evaporative permeation	Ethanol, E85, E70	All ethanol	0	1.501	1.501

CH_4/THC and speciationConstant parameters for Tier 2 vehicles

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

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

Proposed updates to CH_4/THC: Code

- CH_4/THC vary by the same factors as NMOG and VOC
  - processID (start, running, ext. idle, fuel vapor venting, etc)
  - fuelSubTypeID (E0, E5, E10, E85, ULSD diesel, biodiesel, CNG, etc)
  - regClassID (light-duty vehicles, light-duty trucks, light-heavy-duty trucks, heavy heavy-duty trucks, etc.)
  - modelYearGroupID (2007-2009, etc.)
- CH_4/THC no longer to vary by:
  - Vehicle age
  - Source Type (vehicle classification based on activity, e.g. Refuse Truck and Transit Bus)

Calculations using SPECIATE profiles

1. $NMOG = TOG - CH_4$

2. $m_{NMHC} = m_{NMOG} + \rho_{NMHC} \times \sum_{i=1}^{N} \left(\frac{m_{OHCi}}{\rho_{OHCi}} \times RF_{OHCi} \right) - \sum_{i=1}^{N} m_{OHCi}$

3. $THC = NMOG \times \frac{NMHC}{NMOG} + CH_4$

4. $VOC = \mathrm{TOG} - CH_4 - C_2H_2 - C_3H_6O$

5. Calculate ratios CH_4/THC, NMOG/NMHC, VOC/NMHC

NOTE:
Equation 2 is rearranged from Equation 1066.635-1 in the Federal Register. For details on each variable see 40 CFR 1066.635.