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

Appendix N
EPAct NMOG Calculation Protocol

Assessment and Standards Division
Office of Transportation and Air Quality
U.S. Environmental Protection Agency

National Renewable Energy Laboratory
U.S. Department of Energy

Coordinating Research Council

NOTICE

This technical report does not necessarily represent final EPA decisions or positions. It is intended to present technical analysis of issues using data that are currently available. The purpose in the release of such reports is to facilitate the exchange of technical information and to inform the public of technical developments.

EPA United States Environmental Protection Agency

EPA-420-R-13-004
April 2013

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19-Feb-2009

The series of calculations shown here (Equations (1) through (6)) must be performed separately for each test phase (bag). The NMOG mass results can then be weighed in the usual way to form a test cycle composite emission rate.

First we calculate corrected NMHC concentration for dilute exhaust (subscript e) and dilution air (subscript d) as follows:

$$NMHC_e = FIDHC_e - r_{CH4} \cdot CH4_e - r_{MeOH} \cdot MeOH_e - r_{EtOH} \cdot EtOH_e - r_{Pr\,OH} \cdot Pr\,OH_e - r_{AcetHO} \cdot AcetHO_e \quad (1)$$

$$NMHC_d = FIDHC_d - r_{CH4} \cdot CH4_d - r_{MeOH} \cdot MeOH_d - r_{EtOH} \cdot EtOH_d - r_{Pr\,OH} \cdot Pr\,OH_d - r_{AcetHO} \cdot AcetHO_d \quad (2)$$

Note that these values are all as ppmC (so speciation results for EtOH, PrOH, and AcetHO reported in ppm of the particular chemical compound will need to be multiplied by 2 or 3 depending on the number of C atoms in the compound).

The following constant values shall be used for FID response factors:

r_{CH4} = 1.15 ppmC/ppmC (this program)
r_{MeOH} = 0.63 ppmC/ppmC (this program)
r_{EtOH} = 0.74 ppmC/ppmC (this program)
r_{PrOH} = 0.85 ppmC/ppmC (CARB)
r_{FormHO} = 0.00 ppmC/ppmC (various sources)
r_{AcetHO} = 0.51 ppmC/ppmC (this program)

Next, we must calculate the dilution factor to be used in generating the net NMHC concentration:

$$DF = \frac{100 \cdot \left[\frac{x}{x + 0.5y + 3.76 \cdot (x + 0.25y - 0.5z)} \right]}{CO2_e + (NMHC_e + CH4_e + MeOH_e + Pr\,OH_e + EtOH_e + FormHO_e + AcetHO_e + CO_e) \cdot 10^{-4}} \quad (3)$$

The parameters x, y and z in Eq. (3) are coefficients taken from the chemical formula $C_xH_yO_z$ of a test fuel. The procedure to calculate their values is provided in Appendix 2.

Once the DF is determined, we calculate the net NMHC concentration as follows:

$$NMHC_{conc} = NMHC_e - NMHC_d \cdot \left(1 - \frac{1}{DF}\right) \quad (4)$$

Then we compute $NMHC_{mass}$:

$$NMHC_{mass} = V_{mix} \cdot Density_{NMHC} \cdot NMHC_{conc} \cdot 10^{-6} \quad (5)$$

Equations (4) and (5) must be repeated for each emission being considered. V_{mix} is the volume of dilute exhaust collected during a given phase of the test cycle, measured in standard cubic feet. Density is the calculated gas phase density of a particular species treated as a $C_1H_yO_z$ ideal gas.

The following values of gas phase density shall be used:

$Density_{NMHC} = 16.334\ g/ft^3$
$Density_{MeOH} = 37.718\ g/ft^3$
$Density_{EtOH} = 27.115\ g/ft^3$
$Density_{PrOH} = 23.581\ g/ft^3$
$Density_{FormHO} = 35.345\ g/ft^3$
$Density_{AcetHO} = 25.929\ g/ft^3$

To generate the NMOG figure, we need methanol, ethanol, 2-propanol, formaldehyde and acetaldehyde mass emissions as computed using Eq. (4) and (5) based on measured concentration values form the speciation results (as in Eq. (1) and (2)).

Finally, then, NMOG mass emissions can be computed as follows:

$$NMOG_{mass} = NMHC_{mass} + MeOH_{mass} + EtOH_{mass} + PrOH_{mass} + FormHO_{mass} + AcetHO_{mass} \quad (6)$$

Once $NMOG_{mass}$ calculations have been completed for all three phases (cold transient (ct), stabilized (s) and hot transient (ht)) of the LA92 test cycle they, calculate the total weighted NMOG emissions using the following formula:

$$NMOG_{wm} = 0.43 \cdot \left(\frac{NMOG_{mass.ct} + NMOG_{mass.s}}{D_{ct} + D_s} \right) + 0.57 \cdot \left(\frac{NMOG_{mass.ht} + NMOG_{mass.s}}{D_{ht} + D_s} \right) \quad (7)$$

For tests where there is no bag 2 or 3 speciation data, NMOG shall be computed assuming emission levels for oxygenated species in bags 2 and 3 are zero.

Attachment 1

Definitions

$NMHC_e$ – Concentration of NMHC in dilute exhaust sample, ppm C equivalent
$FIDHC_e$ - Uncorrected concentration of HC in dilute exhaust sample as measured by the FID, ppm C equivalent
$CH4_e$ – Concentration of methane in dilute exhaust sample as measured, ppm C equivalent
$MeOH_e$ - Concentration of methanol in dilute exhaust sample as measured, ppm C equivalent
$EtOH_e$ - Concentration of ethanol in dilute exhaust sample as measured, ppm C equivalent
$PrOH_e$ - Concentration of 2-propanol in dilute exhaust sample as measured, ppm C equivalent
$FormHO_e$ - Concentration of formaldehyde in dilute exhaust sample as measured, ppm C equivalent
$AcetHO_e$ - Concentration of acetaldehyde in dilute exhaust sample as measured, ppm C equivalent
$CO2_e$ - Concentration of carbon dioxide in dilute exhaust sample as measured, percent
CO_e - Concentration of carbon monoxide in dilute exhaust sample as measured, ppm
r_{CH4} - FID response to methane, ppmC/ppmC
r_{MeOH} - FID response to methanol, ppmC/ppmC
r_{EtOH} - FID response to ethanol, ppmC/ppmC
r_{PrOH} - FID response to 2-propanol, ppmC/ppmC
r_{FormHO} - FID response to formaldehyde, ppmC/ppmC
r_{AcetHO} - FID response to acetaldehyde, ppmC/ppmC
$NMHC_d$ - NMHC concentration in dilution air, ppm C equivalent
$FIDHC_d$ - Uncorrected HC concentration in dilution air sample as measured by the FID, ppm C equivalent
$CH4_d$ - Concentration of methane in dilution air sample as measured, ppm C equivalent
$MeOH_d$ - Concentration of methanol in dilution air sample as measured, ppm C equivalent
$EtOH_d$ - Concentration of ethanol in dilution air sample as measured, ppm C equivalent
$PrOH_d$ - Concentration of 2-propanol in dilution air sample as measured, ppm C equivalent
$FormHO_d$ - Concentration of formaldehyde in dilution air sample as measured, ppm C equivalent
$AcetHO_d$ - Concentration of acetaldehyde in dilution air sample as measured, ppm C equivalent
$_{DF}$ - Dilution factor
$_x$ - Carbon-to-carbon ratio in formula $C_xH_yO_z$ determined as in Appendix 2 for the fuel used (by definition x=1)
$_y$ - Hydrogen-to-carbon ratio in formula $C_xH_yO_z$ determined as in Appendix 2 for the fuel used
$_z$ - Oxygen-to-carbon ratio in formula $C_xH_yO_z$ determined as in Appendix 2 for the fuel used
X – Carbon mass fraction of the fuel
Y – Hydrogen mass fraction of the fuel
Z – Oxygen mass fraction of the fuel
$NMHC_{conc}$ – Concentration of NMHC in dilute exhaust sample corrected for background, ppm C equivalent
$MeOH_{conc}$ - Concentration of methanol in dilute exhaust sample corrected for background, ppm C equivalent

$EtOH_{conc}$ - Concentration of ethanol in dilute exhaust sample corrected for background, ppm C equivalent
$PrOH_{conc}$ - Concentration of 2-propanol in dilute exhaust sample corrected for background, ppm C equivalent
$FormHO_{conc}$ - Concentration of formaldehyde in dilute exhaust sample corrected for background, ppm C equivalent
$AcetHO_{conc}$ - Concentration of acetaldehyde in dilute exhaust sample corrected for background, ppm C equivalent
V_{mix} - Volume of dilute exhaust collected during a given phase of the test cycle, scf
$Density_{NMHC}$ – Density of NMHC treated as a C_1H_y ideal gas at standard conditions of 293.16°K and 760 mm Hg, g/ft^3
$Density_{MeOH}$ - Density of methanol treated as a $C_1H_yO_z$ ideal gas at standard conditions of 293.16°K and 760 mm Hg, g/ft^3
$Density_{EtOH}$ - Density of ethanol treated as a $C_1H_yO_z$ ideal gas at standard conditions of 293.16°K and 760 mm Hg, g/ft^3
$Density_{PrOH}$ - Density of 2-propanol treated as a $C_1H_yO_z$ ideal gas at standard conditions of 293.16°K and 760 mm Hg, g/ft^3
$Density_{FormHO}$ - Density of formaldehyde treated as a $C_1H_yO_z$ ideal gas at standard conditions of 293.16°K and 760 mm Hg,ft^3
$Density_{AcetHO}$ - Density of acetaldehyde treated as a $C_1H_yO_z$ ideal gas at standard conditions of 293.16°K and 760 mm Hg, g/ft^3
M_{NMHC} - Molecular mass of NMHC treated as a C_1H_y, g/mole, calculated according to the formula provided in Appendix 3
$NMOG_{mass}$ - NMOG mass, g/test phase
$NMHC_{mass}$ - NMHC mass, g/test phase
$MeOH_{mass}$ - Methanol mass, g/test phase
$EtOH_{mass}$ - Ethanol mass, g/test phase
$PrOH_{mass}$ - 2-propanol mass, g/test phase
$FormHO_{mass}$ - Formaldehyde mass, g/test phase
$AcetHO_{mass}$ - Acetaldehyde mass, g/test phase
$NMOG_{wm}$ – Weighted NMOG emissions, g/mile
$NMOG_{mass.ct}$ - NMOG mass emitted during the cold transient phase of the test cycle, g/test phase
$NMOG_{mass.s}$ - NMOG mass emitted during the stabilized phase of the test cycle, g/test phase
$NMOG_{mass.ht}$ - NMOG mass emitted during the hot transient phase of the test cycle, g/test phase
D_{ct} - Distance driven by the test vehicle on a chassis dynamometer during the cold transient phase of the LA92 test cycle, miles
D_s - Distance driven by the test vehicle on a chassis dynamometer during the stabilized phase of the LA92 test cycle, miles
D_{ht} - Distance driven by the test vehicle on a chassis dynamometer during the hot transient phase of the LA92 test cycle, miles

Attachment 2

Calculation of x, y and z Coefficients in Formula $C_xH_yO_z$ Using Fuel C, H and O Content Data

The carbon-to-carbon ratio x in formula $C_xH_yO_z$ by definition equals 1. The hydrogen-to-carbon and oxygen-to-carbon ratios y and z, respectively, can be calculated using the following equations:

$$y = \frac{\frac{Y}{1.008}}{\frac{X}{12.011}} \quad \text{(A2.1)} \qquad \text{and} \qquad z = \frac{\frac{Z}{15.999}}{\frac{X}{12.011}} \quad \text{(A2.2)}$$

where:

X – Carbon mass fraction of the fuel
Y – Hydrogen mass fraction of the fuel
Z – Oxygen mass fraction of the fuel

The values of X, Y and Z will be provided by the EPA for all fuels tested in the EPAct Program.