2014

FEAT Math II

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FEAT Equations for CO, HC and NO.   G. A. Bishop Last updated Feb. 2014.

ASSUMPTIONS:

Fuel C:H ratio is 2 and non-oxygenated. Applies to gasoline and diesel in general.

Fuel is approximated with a mix of Octane and Benzene that averages the molecular formula of CH_2.

Fuel out tailpipe is similar (to make the math simpler we have chosen for the exhaust HC to be a multiple of the input HC) to calibration gas which is propane.

Concentrations are calculated on a dry basis and corrected for any excess air not involved in combustion (these equations are correct for gasoline vehicles, but only the ratios are correct for diesel vehicles) and assume an 8cm path length. For a direct tailpipe comparison for diesel vehicles, the measurement comparison either must consider only the ratios, or must be corrected for the considerable excess oxygen not involved in typical diesel combustion).

Equal amount of seen HC's and unseen HC's in the exhaust (Singer & Harley et al, Environ. Sci Technol. 1998, 32, 3241-3248) Singer factor of 2.

$$CH_2 + m(0.21\ O_2 + 0.79\ N_2) \rightarrow aCO + bH_2O + c(C_3H_6 + inv\ C_3H_6) + dCO_2 + eNO + \left(0.79m - \frac{e}{2}\right) N_2$$

$$Q = \frac{CO}{CO_2} = \frac{a}{d} \qquad Q' = \frac{HC}{CO_2} \qquad Q" = \frac{NO}{CO_2} = \frac{e}{d}$$

by Carbon balance :   a + 6c + d = 1

by Hydrogen balance: 2b + 12c = 2

by Oxygen balance: a + b + 2d + e= 0.42m

Eliminate a: a = dQ   c = dQ'

a + 6c + d = 1   dQ + 6dQ' + d = 1

$$d = \frac{1}{Q + 6Q' + 1}$$

Eliminate b: 2b + 12dQ' = 2 ;   b = 1 - 6dQ'

dQ + b + 2d + e= 0.42m;   dQ + 1 - 6dQ' +2d + e= 0.42m substituting d from above:

$$0.42\,\frac{m}{d} = Q + \frac{1}{d} - 6Q' + 2 + Q" = Q+Q+6Q'+1-6Q'+2+Q" = 2Q + 3 + Q"$$

From the combustion equation the mole fraction of CO_2 is:

$$fCO_2 = \frac{d}{a + 2c + d + e + 0.79m - \frac{e}{2}}$$

divide numerator and denominator by d:

$$fCO_2 = \frac{1}{\frac{a}{d} + 2\frac{c}{d} + 1 + 0.5\frac{e}{d} + 0.79\frac{m}{d}}$$

substituting from above for a/d, c/d and e/d to get:

$$fCO_2 = \frac{1}{Q + 2Q' + 1 + 0.5Q" + 0.79\frac{m}{d}}$$

multiply numerator and denominator by 0.42:

$$fCO_2 = \frac{0.42}{0.42Q + 0.84Q' + 0.42 + 0.21Q" + (0.79)(0.42\frac{m}{d})}$$

substituting from above (0.42 m/d = 2Q + 3 + Q”) leads to:

$$fCO_2 = \frac{0.42}{2.79 + 2Q + 0.84Q' + Q"}$$

from which follows:

$$\%CO_2 = \frac{42}{2.79 + 2Q + 0.84Q' + Q"} = \frac{100}{6.64 + 4.76Q + 2Q' + 2.38Q"}$$

$$\%CO = Q * \%CO_2 \qquad \%HC = Q' * \%CO_2 \qquad \%NO = Q" * \%CO_2$$

Some useful conversions are:

For grams/gallon assume fuel density of 726 g/l, a fuel carbon fraction of 86%, 3.79 l/gallon and for CO 28g/mole; for HC (propane, C_3H_8) 44g/mole for NO 30g/mole; for C 12g/mole:

$$\frac{gmCO}{gal} = \frac{28*Q*0.86*726*3.79}{(1+Q+6Q')*12}$$

$$\frac{gmHC}{gal} = \frac{2*44*Q'*0.86*726*3.79}{(1+Q+6Q')*12}$$

$$\frac{gmNO}{gal} = \frac{30*Q''*0.86*726*3.79}{(1+Q+6Q')*12}$$

We now prefer to use grams of pollutant/kg of fuel because it requires no assumption about the fuel density:

$$\frac{gmCO}{kg} = \frac{28*Q*860}{(1+Q+6Q')*12}$$

$$\frac{gmHC}{kg} = \frac{2*44*Q'*860}{(1+Q+6Q')*12}$$

$$\frac{gmNO}{kg} = \frac{30*Q''*860}{(1+Q+6Q')*12}$$

If you want to express the measured ratios in the units of other molecules, for example gmNO_2/kg since all emitted NO will eventually oxidize in the atmosphere to NO_2, you only have to change the molecular weight of the species in the appropriate equation.

Derivation for methane powered vehicles:

ASSUMPTIONS:

Singer factor of 3.13.

$$CH_4 + m(0.21\ O_2 + 0.79\ N_2) \rightarrow$$
$$aCO + bH_2O + c(CH_4 + 2.13\ CH_4) + dCO_2 + eNO + \left(0.79m - \frac{e}{2}\right) N_2$$

$$Q = \frac{CO}{CO_2} = \frac{a}{d} \qquad Q' = \frac{HC}{CO_2} \qquad Q" = \frac{NO}{CO_2} = \frac{e}{d}$$

by Carbon balance : a + 3.13c + d = 1

by Hydrogen balance: 2b + 12.52c = 4

by Oxygen balance: a + b + 2d + e= 0.42m

Eliminate a: a = dQ c = dQ'

a + 3.13c + d = 1 dQ + 3.13dQ' + d = 1

$$d = \frac{1}{Q + 3.13Q' + 1}$$

Eliminate b: 2b + 12.52dQ' = 4 b = 2 – 6.26dQ'

dQ + b + 2d + e= 0.42m; dQ + 2 – 6.26dQ' +2d + e= 0.42m

substituting d from above:

$$0.42\ \frac{m}{d} = Q + \frac{2}{d} - 6.26Q' + 2 + Q" = Q+2+2Q+6.26Q'-6.26Q'+2+Q" = 3Q + 4 + Q"$$

from the combustion equation the mole fraction of CO_2 is:

$$fCO_2 = \frac{d}{a + 3.13c + d + e + 0.79m - \frac{e}{2}}$$

divide numerator and denominator by d:

$$fCO_2 = \frac{1}{\frac{a}{d} + 3.13\frac{c}{d} + 1 + 0.5\frac{e}{d} + 0.79\frac{m}{d}}$$

Substituting from above for a/d, c/d and e/d to get:

$$fCO_2 = \frac{1}{Q + 3.13Q' + 1 + 0.5Q" + 0.79\frac{m}{d}}$$

Multiply numerator and denominator by 0.42:

$$fCO_2 = \frac{0.42}{0.42Q + 1.32Q' + 0.42 + 0.21Q" + (0.79)(0.42\frac{m}{d})}$$

Substituting from above (0.42m/d = 3Q + 4 + Q")

$$fCO_2 = \frac{0.42}{3.58 + 2.79Q + 1.32Q' + Q"}$$

From which follows:

$$\%CO_2 = \frac{42}{3.58 + 2.79Q + 1.32Q' + Q"} = \frac{100}{8.52 + 6.64Q + 3.14Q' + 2.38Q"}$$

$$\%CO = Q * \%CO_2 \qquad \%HC = Q' * \%CO_2 \qquad \%NO = Q" * \%CO_2$$

For grams/gallon for LNG assume fuel density of 450 g/l, a fuel carbon fraction of 75%, 3.79 l/gallon and for CO 28g/mole; for HC (methane, CH_4) 16g/mole for NO 30g/mole; for C 12g/mole:

$$\frac{gmCO}{gal} = \frac{28 * Q * 0.75 * 450 * 3.79}{(1 + Q + 3.13Q') * 12} \qquad \frac{gmCO}{kg} = \frac{28 * Q * 750}{(1 + Q + 3.13Q') * 12}$$

$$\frac{gmHC}{gal} = \frac{3.13 * 16 * Q' * 0.75 * 450 * 3.79}{(1 + Q + 3.13Q') * 12} \qquad \frac{gmHC}{kg} = \frac{3.13 * 16 * Q' * 750}{(1 + Q + 3.13Q') * 12}$$

$$\frac{gmNO}{gal} = \frac{30 * Q" * 0.75 * 450 * 3.79}{(1 + Q + 3.13Q') * 12} \qquad \frac{gmNO}{kg} = \frac{30 * Q" * 750}{(1 + Q + 3.13Q') * 12}$$