WHEN YOU NEED TO BE SURE

CyFlex® Knowledge Article

Exhaust Gas Composition

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To a good approximation, for overall lean combustion of an ideal fuel with “standard” moist air, the reaction equation may be written as:

$$(C\,H_\beta O_\gamma N_\delta S_\eta) \quad + \quad a\left(wO_2 + xN_2 + yA + zCO_2\right) \quad + \quad bH_2O$$
$$\Rightarrow \quad cH_2O + dCO_2 + eO_2 + f\,N_2 + gA + hS \qquad \text{ec.1}$$

where:

a is the number of moles of dry air per mole of fuel carbon.

β, γ, δ, and η are respectively, the number of moles of hydrogen, oxygen, nitrogen and sulfur atoms per mole of fuel carbon.

w, x, y, and *z* are respectively the number of moles of oxygen, nitrogen, argon and carbon dioxide per mole of dry combustion air.

b is the number of moles of water vapor per mole of fuel carbon.

c, d, e, f, g, and *h* are respectively the number of moles of water vapor, carbon dioxide, oxygen, nitrogen, argon, and sulfur in the exhaust per mole of fuel carbon.

For natural gas, the composition is measured with a gas chromatograph and provided in the form of mole fractions, y_x, for methane, ethane, propane, isobutane, nbutane, pentanes, hexanes and higher, hydrogen, carbon monoxide, nitrogen, oxygen, carbon dioxide and hydrogen sulfide. $\tilde{\alpha}$, $\tilde{\beta}$, $\tilde{\gamma}$, $\tilde{\delta}$, and $\tilde{\eta}$, the number of moles of carbon, hydrogen, oxygen, nitrogen, and sulfur atoms per mole of fuel may be determined from:

$$\tilde{\alpha} = y_{methane} + 2y_{ethane} + 3y_{propane} + 4y_{isobutane} + 4y_{nbutane} + 5y_{pentanes} + 6y_{hexanes} + y_{carbon\ monoxide} + y_{carbon\ dioxide} \qquad \text{ec.2}$$

$$\tilde{\beta} = 4y_{methane} + 6y_{ethane} + 8y_{propane} + 10y_{isobutane} + 10y_{nbutane} + 12y_{pentanes} + 14y_{hexanes} + 2y_{hydrogen} + 2y_{hydrogen\ sulfide} \qquad \text{ec.3}$$

$$\tilde{\gamma} = y_{carbon\ monoxide} + 2y_{oxygen} + 2y_{carbon\ dioxide} \qquad \text{ec.4}$$

$$\tilde{\delta} = 2y_{nitrogen} \qquad \text{ec.5}$$

$$\tilde{\eta} = y_{hydrogen\ sulfide} \qquad \text{ec.6}$$

Note: The “standard” moist air mentioned above was based on a customer’s standard.

To convert to a moles-per-mole of fuel carbon basis:

$$1 = \frac{\tilde{\alpha}}{\tilde{\alpha}}, \quad \beta = \frac{\tilde{\beta}}{\tilde{\alpha}}, \quad \gamma = \frac{\tilde{\gamma}}{\tilde{\alpha}}, \quad \delta = \frac{\tilde{\delta}}{\tilde{\alpha}}, \quad \eta = \frac{\tilde{\eta}}{\tilde{\alpha}} \qquad \text{ec.7}$$

For diesel fuel, the number of moles of oxygen, nitrogen and sulfur are typically considered to be zero. β may be determined from the measured fuel hydrogen and carbon weight fractions and the molecular weights, *M*, of carbon and hydrogen using:

$$\beta = \frac{fuel\ hydrogen\ wt\ fraction}{fuel\ carbon\ wt\ fraction} \times \frac{M_C}{M_H} \qquad \text{ec.8}$$

w, x, y, and *z,* the number of moles of oxygen, nitrogen, argon, and carbon dioxide per mole of dry "standard" combustion air are:

$$w = 0.20946$$
$$x = 0.78087$$
$$y = 0.00934$$
$$z = 0.00033$$

a, the number of moles of dry combustion air per mole of fuel carbon, can be calculated based on measurements of fuel and dry air mass flow using:

$$\frac{dry\ air\ mass\ \ flow\ rate}{fuel\ mass\ \ flow\ rate} = \left.\frac{A}{F}\right|_{dry} = \frac{a\ M_{air}}{M_{fuel}} \qquad \text{ec.9}$$

which may be solved for *a:*

$$a = \left.\frac{A}{F}\right|_{dry} \frac{M_{fuel}}{M_{air}} \qquad \text{ec.10}$$

The molecular weight of "standard" air is:

M_{air} = 28.9646

Note: The "standard" combustion air and molecular weight of "standard" air mentioned above were based on a customer's standards.

For natural gas, the molecular weight on a per mole of fuel carbon basis is given by:

$$M_{fuel} = M_C + \beta M_H + \gamma M_O + \delta M_N + \eta M_S \qquad \text{ec.11}$$

For diesel fuel, we have:

$$M_{fuel} = M_C + \beta M_H \qquad \text{ec.12}$$

b, the number of moles of water vapor per mole of dry combustion air, can be determined based on vapor and barometric pressure measurements. The mole fraction of water vapor in the wet combustion air is equal to the partial pressure of water vapor, so:

$$\frac{P_{vap}}{P_{bar}} = \frac{b}{b+a} \qquad \text{ec.13}$$

Solving for *b* in terms of the measured pressures gives:

$$b = a\frac{P_{vap}}{P_{bar} - P_{vap}}$$ ec.14

a can also be calculated based on measurements of fuel and wet air mass flow using:

$$\frac{wet\ air\ mass\ flow\ rate}{fuel\ mass\ flow\ rate} = \left.\frac{A}{F}\right|_{wet} = \frac{a\,M_{air} + b\,M_{H_2O}}{M_{fuel}}$$ ec.15

Substituting ec.14 gives:

$$\left.\frac{A}{F}\right|_{wet} = a\left[\frac{M_{air} + \frac{P_{vap}}{P_{bar} - P_{vap}}M_{H_2O}}{M_{fuel}}\right]$$ ec.16

which may be solved for *a:*

$$a = \left.\frac{A}{F}\right|_{wet}\left[\frac{M_{fuel}}{M_{air} + \frac{P_{vap}}{P_{bar} - P_{vap}}M_{H_2O}}\right]$$ ec.17

Atom balances yield the following equations:

$C:$ ec.18

$$1 + a\,z = d$$

$H:$ ec.19

$$\beta + 2b = 2c$$

$O:$ ec.20

$$\gamma + 2aw + 2az + b = c + 2d + 2e$$

$N:$ ec.21

$$\delta + 2ax = 2f$$

$S:$ ec.22

$$\eta = h$$

$A:$ ec.23

$$ay = g$$

Solving the atom balance equations for the products in terms of *a*, *b*, α, β, γ, δ, η, *w*, *x*, *y* and *z* gives:

$$c = b + \frac{\beta}{2} \quad \text{ec.24}$$

$$d = az + 1 \quad \text{ec.25}$$

$$e = \frac{\gamma}{2} + aw - \frac{\beta}{4} - 1 \quad \text{ec.26}$$

$$f = \frac{\delta}{2} + ax \quad \text{ec.27}$$

$$g = ay \quad \text{ec.28}$$

$$h = \eta \quad \text{ec.29}$$

The total number of moles of exhaust gas per mole of fuel carbon may be determined from:

$$\begin{aligned} c + d + e + f + g + h &= b + \beta/2 + az + 1 + \gamma/2 + aw - \beta/4 - 1 + \delta/2 + ax + ay + \eta \\ &= a(w + x + y + z) + b + \beta/4 + \gamma/2 + \delta/2 + \eta \\ &= a + b + \beta/4 + \gamma/2 + \delta/2 + \eta \end{aligned} \quad \text{ec.30}$$

The mole fractions of the exhaust gases on a wet basis are:

$$y_{H_2O,wet} = \frac{c}{c + d + e + f + g + h} = \frac{b + \beta/2}{a + b + \beta/4 + \gamma/2 + \delta/2 + \eta} \quad \text{ec.31}$$

$$y_{CO_2,wet} = \frac{d}{c + d + e + f + g + h} = \frac{az + 1}{a + b + \beta/4 + \gamma/2 + \delta/2 + \eta} \quad \text{ec.32}$$

$$y_{O_2,wet} = \frac{e}{c + d + e + f + g + h} = \frac{\gamma/2 + aw - \beta/4 - 1}{a + b + \beta/4 + \gamma/2 + \delta/2 + \eta} \quad \text{ec.33}$$

$$y_{N_2,wet} = \frac{f}{c + d + e + f + g + h} = \frac{ax + \delta/2}{a + b + \beta/4 + \gamma/2 + \delta/2 + \eta} \quad \text{ec.34}$$

$$y_{A,wet} = \frac{g}{c + d + e + f + g + h} = \frac{ay}{a + b + \beta/4 + \gamma/2 + \delta/2 + \eta} \quad \text{ec.35}$$

$$y_{S,wet} = \frac{h}{c + d + e + f + g + h} = \frac{\eta}{a + b + \beta/4 + \gamma/2 + \delta/2 + \eta} \quad \text{ec.36}$$

The exhaust molecular weight is:

$$M_{exh} = y_{CO_2} M_{CO_2} + y_{H_2O} M_{H_2O} + y_{O_2} M_{O_2} + y_{N_2} M_{N_2} + y_A M_A + y_S M_S \quad \text{ec.37}$$

Some of the exhaust gas concentrations are typically measured after all or nearly all of the water vapor is removed. The exhaust mole fractions on a dry basis are:

$$y_{H_2O,dry} = 0 \qquad \text{ec.38}$$

$$y_{CO_2,dry} = \frac{d}{d+e+f+g+h} = \frac{az+1}{a-\beta/4+\gamma/2+\delta/2+\eta} \qquad \text{ec.39}$$

$$y_{O_2,dry} = \frac{e}{d+e+f+g+h} = \frac{\gamma/2+aw-\beta/4-1}{a-\beta/4+\gamma/2+\delta/2+\eta} \qquad \text{ec.40}$$

$$y_{N_2,dry} = \frac{f}{d+e+f+g+h} = \frac{ax+\delta/2}{a-\beta/4+\gamma/2+\delta/2+\eta} \qquad \text{ec.41}$$

$$y_{A,dry} = \frac{g}{d+e+f+g+h} = \frac{ay}{a-\beta/4+\gamma/2+\delta/2+\eta} \qquad \text{ec.42}$$

$$y_{S,dry} = \frac{h}{d+e+f+g+h} = \frac{\eta}{a-\beta/4+\gamma/2+\delta/2+\eta} \qquad \text{ec.43}$$

To convert the measured dry mole fraction of some minor species such as NO_X or CO to a wet basis it is necessary to multiply by the factor:

$$\frac{d+e+f+g+h}{c+d+e+f+g+h} = 1-\frac{c}{c+d+e+f+g+h} = 1-y_{H_2O,wet} \qquad \text{ec.44}$$

$$= 1-\frac{b+\beta/2}{a+b+\beta/4+\gamma/2+\delta/2+\eta}$$