WHEN YOU NEED TO BE SURE

CyFlex® Knowledge Article

Burned Gas Composition

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Basic Combustion Equation

In a strict thermodynamic sense, the equilibrium burned gas composition can be uniquely defined by specifying the atom ratios C:H:O:N:A:S and the burned gas pressure and temperature. If we simplify things by assuming that pressure effects are small and considering only equilibrium products at low temperature (< 1000 K), the combustion of two or more gas streams may be represented by the reaction equation

$$a\left(y_{A,a}A + y_{B,a}B + y_{C,a}C + \ldots \right) \; + \; b\left(y_{A,b}A + y_{B,b}B + y_{C,b}C + \ldots \right) \; + \; \ldots \; \Rightarrow \quad \text{bgc.1}$$
$$\alpha\, H_2O + \beta\, CO_2 + \gamma\, O_2 + \delta\, CO + \eta\, H_2 + \lambda\, N_2 + \psi\, A + \omega\, S$$

where

$a, b, \ldots \; = \;$ *mole flow rate of given stream.*

$y_{X,z} \; = \;$ *mole fraction of component X in stream z.*

$\alpha, \beta, \gamma, \ldots \; = \;$ *mole flow rate of given burned gas stream component.*

Molar Flow Rates

The molar flow rates of the reactant streams can be calculated from

$$a = \frac{\dot{m}_a}{M_a} \qquad b = \frac{\dot{m}_b}{M_b} \qquad \ldots \qquad \text{bgc.2}$$

where

$\dot{m}_z \; = \;$ *mass flow rate of stream z.*

$M_z \; = \;$ *molecular weight of stream z.*

Atom Balances

Atom balances yield the following set of equations which can be solved to determine the flow rates of the burned gas components:

C:

$$\left.\begin{array}{l} a\, w_{C,A}\, y_{A,a} + a\, w_{C,B}\, y_{B,a} + a\, w_{C,C}\, y_{C,a} + \ldots \\ b\, w_{C,A}\, y_{A,b} + b\, w_{C,B}\, y_{B,b} + b\, w_{C,C}\, y_{C,b} + \ldots \\ \ldots \end{array}\right\} = \Pi \qquad \text{bgc.3}$$
$$= \beta + \delta$$

H:

$$\left.\begin{array}{l} a\,w_{H,A}\,y_{A,a} + a\,w_{H,B}\,y_{B,a} + a\,w_{H,C}\,y_{C,a} + \dots \\ b\,w_{H,A}\,y_{A,b} + b\,w_{H,B}\,y_{B,b} + b\,w_{H,C}\,y_{C,b} + \dots \\ \dots \end{array}\right\} = \Theta \\ = 2\alpha + 2\eta \qquad \text{bgc.4}$$

O:

$$\left.\begin{array}{l} a\,w_{O,A}\,y_{A,a} + a\,w_{O,B}\,y_{B,a} + a\,w_{O,C}\,y_{C,a} + \dots \\ b\,w_{O,A}\,y_{A,b} + b\,w_{O,B}\,y_{B,b} + b\,w_{O,C}\,y_{C,b} + \dots \\ \dots \end{array}\right\} = \Sigma \\ = \alpha + 2\beta + 2\gamma + \delta \qquad \text{bgc.5}$$

N:

$$\left.\begin{array}{l} a\,w_{N,A}\,y_{A,a} + a\,w_{N,B}\,y_{B,a} + a\,w_{N,C}\,y_{C,a} + \dots \\ b\,w_{N,A}\,y_{A,b} + b\,w_{N,B}\,y_{B,b} + b\,w_{N,C}\,y_{C,b} + \dots \\ \dots \end{array}\right\} = \Delta \\ = 2\lambda \qquad \text{bgc.6}$$

A:

$$\left.\begin{array}{l} a\,w_{A,A}\,y_{A,a} + a\,w_{A,B}\,y_{B,a} + a\,w_{A,C}\,y_{C,a} + \dots \\ b\,w_{A,A}\,y_{A,b} + b\,w_{A,B}\,y_{B,b} + b\,w_{A,C}\,y_{C,b} + \dots \\ \dots \end{array}\right\} = \Omega \\ = \psi \qquad \text{bgc.7}$$

S:

$$\left.\begin{array}{l} a\,w_{S,A}\,y_{A,a} + a\,w_{S,B}\,y_{B,a} + a\,w_{S,C}\,y_{C,a} + \dots \\ b\,w_{S,A}\,y_{A,b} + b\,w_{S,B}\,y_{B,b} + b\,w_{S,C}\,y_{C,b} + \dots \\ \dots \end{array}\right\} = \Lambda \\ = \omega \qquad \text{bgc.8}$$

where:

$$w_{V,X} = \text{moles of } V \text{ atoms per mole of component } X$$
$$(\text{eg. } 2 \text{ moles of hydrogen atoms per mole of } H_2O)$$

Stoichiometry

At this point, we have arrived at a set of six equations in eight unknowns. To add more equations or further simplify the ones we have, we need to know whether there is enough oxygen present to react with the hydrogen and carbon to burn completely to form carbon dioxide and water vapor. If we were just dealing with mixtures of fuel and fresh air, we could make this determination by considering the “equivalence ratio” or “stoichiometry” of the mixture. For the more general mixtures we are dealing with here, we are forced to directly examine the weighted ratio of carbon and hydrogen atoms to oxygen atoms.

Lean or Stoichiometric Combustion

If we have just the right amount of oxygen to form what would commonly be called a “stoichiometric” mixture, then

$$\gamma = 0, \quad \delta = 0 \quad and \quad \eta = 0 \qquad \text{bgc.9}$$

and we can write

$$\left.\begin{aligned} \Pi &= \beta \\ \Theta &= 2\alpha \\ \Sigma &= \alpha + 2\beta \end{aligned}\right\} \Rightarrow \frac{\frac{\Theta}{2} + 2\Pi}{\Sigma} = 1 \qquad \text{bgc.10}$$

For a lean mixture, there is excess oxygen, so:

$$\boxed{\frac{\frac{\Theta}{2} + 2\Pi}{\Sigma} < 1, \quad \delta = 0 \quad and \quad \eta = 0} \qquad \text{bgc.11}$$

For either a “stoichiometric” or lean mixture, the set of equations reduces to

$$\beta = \Pi \qquad \text{bgc.12}$$

$$\alpha = \frac{\Theta}{2} \qquad \text{bgc.13}$$

$$\gamma = \frac{\Sigma - \alpha - 2\beta}{2} = \frac{\Sigma}{2} - \frac{\Theta}{4} - \Pi \qquad \text{bgc.14}$$

$$\lambda = \frac{\Delta}{2} \qquad \text{bgc.15}$$

$$\psi = \Omega \qquad \text{bgc.16}$$

$$\omega = \Lambda \qquad \text{bgc.17}$$

Rich Combustion

For the rich case, there is insufficient oxygen, so

$$\frac{\frac{\Theta}{2} + 2\Pi}{\Sigma} > 1 \quad and \quad \gamma = 0$$ bgc.18

We now need to consider an additional reaction

$$CO_2 + H_2 \Leftrightarrow CO + H_2O$$ bgc.19

The equilibrium constant for the reaction is given by

$$\mathrm{K}(\mathrm{T}) = \frac{\alpha\,\delta}{\beta\,\eta}$$ bgc.20

where K(T) may be approximated by

$$\ln K(T) = 2.743 - \frac{1.761\times10^{3}}{T} - \frac{1.611\times10^{6}}{T^{2}} + \frac{0.2803\times10^{9}}{T^{3}}$$ bgc.21

where T is in Kelvin. We can then write

$$\hat{a} = K - 1$$ bgc.22

$$\hat{b} = -K\Pi - \frac{K\Theta}{2} + K\Sigma - 2\Pi K - \Sigma + 2\Pi$$ bgc.23

$$\hat{c} = \frac{K\Pi\Theta}{2} - K\Pi\Sigma + 2K\Pi^{2}$$ bgc.24

$$\delta = \frac{-\hat{b} - \sqrt{\hat{b}^{2} - 4\hat{a}\,\hat{c}}}{2\hat{a}}$$ bgc.25

$$\beta = \Pi - \delta$$ bgc.26

$$\alpha = \Sigma - \delta - 2\beta$$ bgc.27

$$\eta = \frac{\Theta}{2} - \alpha$$ bgc.28

$$\lambda = \frac{\Delta}{2}$$ bgc.29

$$\psi = \Omega$$ bgc.30

$$\omega = \Lambda$$ bgc.31

Wet Exhaust Gas Mole Fractions

Once the burned gas composition is determined, the mole fractions of the burned gas components can be calculated from

$$y_{H_2O,burned} = \frac{\alpha}{\alpha+\beta+\gamma+\delta+\eta+\lambda+\psi+\omega} \quad \text{bgc.32}$$

$$y_{CO_2,burned} = \frac{\beta}{\alpha+\beta+\gamma+\delta+\eta+\lambda+\psi+\omega} \quad \text{bgc.33}$$

$$y_{O_2,burned} = \frac{\gamma}{\alpha+\beta+\gamma+\delta+\eta+\lambda+\psi+\omega} \quad \text{bgc.34}$$

$$y_{CO,burned} = \frac{\delta}{\alpha+\beta+\gamma+\delta+\eta+\lambda+\psi+\omega} \quad \text{bgc.35}$$

$$y_{H_2,burned} = \frac{\eta}{\alpha+\beta+\gamma+\delta+\eta+\lambda+\psi+\omega} \quad \text{bgc.36}$$

$$y_{N_2,burned} = \frac{\lambda}{\alpha+\beta+\gamma+\delta+\eta+\lambda+\psi+\omega} \quad \text{bgc.37}$$

$$y_{A,burned} = \frac{\psi}{\alpha+\beta+\gamma+\delta+\eta+\lambda+\psi+\omega} \quad \text{bgc.38}$$

$$y_{S,burned} = \frac{\omega}{\alpha+\beta+\gamma+\delta+\eta+\lambda+\psi+\omega} \quad \text{bgc.39}$$

Dry Exhaust Gas Mole Fractions

Many of the instruments used to measure species concentrations in the exhaust gas are sensitive to the presence of water vapor. To prevent equipment damage and interference with the measurement, the water vapor is removed and the measurements are made on a “dry” basis. The expected mole fractions (concentrations) on a dry basis may be determined by multiplying by the wet to dry conversion factor

$$\frac{\alpha+\beta+\gamma+\delta+\eta+\lambda+\psi+\omega}{\beta+\gamma+\delta+\eta+\lambda+\psi+\omega} = \frac{1}{1-y_{H_2O,burned}} \qquad \text{bgc.40}$$

So on a dry basis, the exhaust mole fractions are given by

$$y_{H_2O,burned,dry} = 0 \qquad \text{bgc.41}$$

$$y_{CO_2,burned,dry} = \frac{\beta}{\beta+\gamma+\delta+\eta+\lambda+\psi+\omega} \qquad \text{bgc.42}$$

$$y_{O_2,burned,dry} = \frac{\gamma}{\beta+\gamma+\delta+\eta+\lambda+\psi+\omega} \qquad \text{bgc.43}$$

$$\vdots$$

Burned Gas Molecular Weight

The burned gas molecular weight is given by

$$M_{burned} = y_{H_2O,burned} M_{H_2O} + y_{CO_2,burned} M_{CO_2} + y_{O_2,burned} M_{O_2} + y_{CO,burned} M_{CO} + y_{H_2,burned} M_{H_2} + y_{N_2,burned} M_{N_2} + y_{A,burned} M_A + y_{S,burned} M_S \qquad \text{bgc.44}$$

Burned Gas Mass Flow Rate

The burned gas mass flow rate is simply the sum of the reactant mass flow rates

$$\dot{m}_{burned} = \dot{m}_a + \dot{m}_b + \cdots \qquad \text{bgc.45}$$