CyFlex® Knowledge Article

Simplified Burned Gas Composition

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Simplifying Assumptions

The combustion of diesel fuel with wet combustion air is still the dominant burning process at the Tech Center. The general equations presented in the *Burned Gas Composition* document can be greatly simplified and then solved in closed form to clarify the relationships between the inputs and calculated outputs. The simplifying assumptions are:

1. There are two reactant streams - diesel fuel and wet combustion air.
2. The ratio of wet combustion air mass flow to fuel mass flow is known.
3. Both the vapor pressure of the wet combustion air and the barometric pressure are known.
4. We know either the hydrogen and carbon weight fractions for the fuel or the molar hydrogen to carbon ratio.
5. The combustion process is overall lean.
6. The amount of sulfur in the fuel is negligible.

Basic Combustion Equation

Given these simplifying assumptions and the developments presented in the *Reactant Stream Composition and Molecular Weight* and *Reactant Stream Flow Rates* sections of *the Burned Gas Composition* document, the reaction equation:

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

can be reduced to:

$$CH_{\tau'} \; + \; b\left[\, y_{dry\ air,wet\ air}\left(y_{O_2,dry\ air}O_2 + y_{N_2,dry\ air}N_2 + y_{Ar,dry\ air}Ar + y_{CO_2,dry\ air}CO_2 \right) \; + \right.$$
$$\left. y_{H_2O,wet\ air}H_2O \,\right] \; \Rightarrow \; \alpha\, H_2O + \beta\, CO_2 + \gamma\, O_2 + \lambda\, N_2 + \psi\, A$$

Atom Balances

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

C:

$$1 \; + \; b\, y_{dry\ air,wet\ air}\; y_{CO_2,dry\ air} \; = \; \Pi$$

$$= \; \beta$$

H:

$$\tau' \; + \; b(2)\, y_{H_2O,wet\ air} \; = \; \Theta$$

$$= \; 2\alpha$$

O:

$$b\left[y_{dry\ air,wet\ air}\left(2\,y_{O_2,dry\ air} + 2\,y_{CO_2,dry\ air}\right) + y_{H_2O,wet\ air}\right] = \Sigma$$

$$= \alpha + 2\beta + 2\gamma$$

N:

$$b\,y_{dry\ air,wet\ air}\,(2)\,y_{N_2,dry\ air} = \Delta$$

$$= 2\lambda$$

A:

$$b\,y_{dry\ air,wet\ air}\;y_{Ar,dry\ air} = \Omega$$

$$= \psi$$

These equations reduce to:

$$\beta = \Pi$$

$$= 1 + b\,y_{dry\ air,wet\ air}\;y_{CO_2,dry\ air}$$

$$\alpha = \frac{\Theta}{2}$$

$$= \frac{\tau'}{2} + b\,y_{H_2O,wet\ air}$$

$$\gamma = \frac{\Sigma - \alpha - 2\beta}{2} = \frac{\Sigma}{2} - \frac{\Theta}{4} - \Pi$$

$$= b\left[y_{dry\ air,wet\ air}\left(y_{O_2,dry\ air} + y_{CO_2,dry\ air}\right) + \frac{y_{H_2O,wet\ air}}{2}\right] - \frac{\tau'}{4} - \frac{b\,y_{H_2O,wet\ air}}{2} - 1 - b\,y_{dry\ air,wet\ air}\;y_{CO_2,dry\ air}$$

$$= b\,y_{dry\ air,wet\ air}\;y_{O_2,dry\ air} - \frac{\tau'}{4} - 1$$

$$\lambda = \frac{\Delta}{2}$$

$$= b\, y_{dry\ air,wet\ air}\ y_{N_2,dry\ air}$$

$$\psi = \Omega$$

$$= b\, y_{dry\ air,wet\ air}\ y_{Ar,dry\ air}$$

Wet Exhaust Gas Mole Fractions

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

$$\begin{aligned}
\alpha+\beta+\gamma+\lambda+\psi &= \left(b\, y_{H_2O,wet\ air} + \frac{\tau'}{2}\right) + \left(b\, y_{dry\ air,wet\ air}\ y_{CO_2,dry\ air} + 1\right) + \\
&\quad \left(b\, y_{dry\ air,wet\ air}\ y_{O_2,dry\ air} - \frac{\tau'}{4} - 1\right) + \\
&\quad \left(b\, y_{dry\ air,wet\ air}\ y_{N_2,dry\ air}\right) + \left(b\, y_{dry\ air,wet\ air}\ y_{Ar,dry\ air}\right) \\
&= b\left[y_{dry\ air,wet\ air}\left(y_{O_2,dry\ air} + y_{N_2,dry\ air} + y_{Ar,dry\ air} + y_{CO_2,dry\ air}\right) + \right. \\
&\quad \left. y_{H_2O,wet\ air}\right] + \frac{\tau'}{4} \\
&= b + \tau'/4
\end{aligned}$$

$$y_{H_2O,burned} = \frac{\alpha}{\alpha+\beta+\gamma+\delta+\eta+\lambda+\psi+\omega} = \frac{b\, y_{H_2O,wet\ air} + \tau'/2}{b + \tau'/4}$$

$$y_{CO_2,burned} = \frac{\beta}{\alpha+\beta+\gamma+\delta+\eta+\lambda+\psi+\omega} = \frac{b\, y_{dry\ air,wet\ air}\ y_{CO_2,dry\ air} + 1}{b + \tau'/4}$$

$$y_{O_2,burned} = \frac{\gamma}{\alpha+\beta+\gamma+\delta+\eta+\lambda+\psi+\omega} = \frac{b\, y_{dry\ air,wet\ air}\ y_{O_2,dry\ air} - \tau'/4 - 1}{b + \tau'/4}$$

$$y_{N_2,burned} = \frac{\lambda}{\alpha+\beta+\gamma+\delta+\eta+\lambda+\psi+\omega} = \frac{b\, y_{dry\ air,wet\ air}\ y_{N_2,dry\ air}}{b + \tau'/4}$$

$$y_{A,burned} = \frac{\psi}{\alpha+\beta+\gamma+\delta+\eta+\lambda+\psi+\omega} = \frac{b\, y_{dry\ air,wet\ air}\ y_{Ar,dry\ air}}{b + \tau'/4}$$

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:

$$\frac{\alpha+\beta+\gamma+\lambda+\psi}{\beta+\gamma+\lambda+\psi} = \frac{1}{1-y_{H_2O,burned}} = \frac{b + \tau'/4}{b\left(1-y_{H_2O,wet\ air}\right)-\tau'/4}$$

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

$$y_{H_2O,burned,dry} = 0$$

$$y_{CO_2,burned,dry} = \frac{\beta}{\beta+\gamma+\delta+\eta+\lambda+\psi+\omega} = \frac{b\,y_{dry\ air,wet\ air}\,y_{CO_2,dry\ air}+1}{b\left(1-y_{H_2O,wet\ air}\right)-\tau'/4}$$

$$y_{O_2,burned,dry} = \frac{\gamma}{\beta+\gamma+\delta+\eta+\lambda+\psi+\omega} = \frac{b\,y_{dry\ air,wet\ air}\,y_{O_2,dry\ air}-\tau'/4-1}{b\left(1-y_{H_2O,wet\ air}\right)-\tau'/4}$$

$$\vdots$$

Burned Gas Molecular Weight

The burned gas molecular weight is given by:

$$\begin{aligned} M_{burned} &= y_{H_2O,burned}M_{H_2O} + y_{CO_2,burned}M_{CO_2} + y_{O_2,burned}M_{O_2} + \\ &\quad y_{N_2,burned}M_{N_2} + y_{A,burned}M_A \end{aligned}$$

Burned Gas Flow Rate

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

$$\dot{m}_{burned} = \dot{m}_a + \dot{m}_b + \cdots$$

Reactant Stream Composition and Molecular Weight

Given our initial assumptions, the reactant stream composition and molecular weights are defined by the following:

Dry Air

The concentrations of oxygen, nitrogen, argon, and carbon dioxide in dry "Cummins standard" combustion air are assumed to be (http://www.ctc.cummins.com/ctc-fe/tsfe/teams/stdcal/aircomp.htm):

$$y_{O_2,dry\ air} = 0.20946$$

$$y_{N_2,dry\ air} \quad = \quad 0.78087$$

$$y_{Ar,dry\ air} \quad = \quad 0.00934$$

$$y_{CO_2,dry\ air} \quad = \quad 0.00033$$

The molecular weight of “Cummins standard” air is
$M_{air,dry}$ = 28.9646

Wet Air

The number of moles of dry air per mole of wet combustion air $y_{dry\ air,wet\ air}$, and the number of moles of water vapor per mole of wet combustion air, $y_{H_2O,wet\ air}$, can be calculated based on vapor and barometric pressure measurements using:

$$y_{dry\ air,wet\ air} \quad = \quad \frac{P_{bar} - P_{vap}}{P_{bar}} \qquad \text{gcls.13}$$

and

$$y_{H_2O,wet\ air} \quad = \quad \frac{P_{vap}}{P_{bar}} \qquad \text{gcls.13}$$

The molecular weight of wet combustion air is given by:

$$\begin{aligned} M_{wet\ air} &= y_{dry\ air,wet\ air}\, M_{dry\ air} + y_{H_2O,wet\ air}\, M_{H_2O} \\ &= \frac{\left(P_{bar} - P_{vap}\right) M_{air,dry} + P_{vap}\, M_{H_2O}}{P_{bar}} \end{aligned} \qquad \text{gcls.13}$$

Diesel Fuel

The hydrogen to carbon mole ratio, τ', can be from measured fuel hydrogen and carbon weight fractions and the molecular weights of carbon and hydrogen atoms using:

$$\tau' \quad = \quad \frac{\tau}{\sigma} \quad = \quad \frac{fuel\ hydrogen\ wt\ fraction}{fuel\ carbon\ wt\ fraction} \quad \times \quad \frac{M_C}{M_H} \qquad \text{gcls.7}$$

If measured fuel hydrogen and carbon weight fractions are not available, the hydrogen to carbon ratio is often assumed to be either 1.85 or 1.80.

The molecular weight of diesel fuel on a per mole of fuel carbon basis is given by:

$$M_{diesel} \quad = \quad M_C + \tau' M_H \qquad \text{gcls.8}$$

Reactant Stream Flow Rates

Since we want to work on a moles of reactant per mole of fuel carbon basis, we set the molar flow rate of fuel, *a*, to:

$$a = 1$$

and find that:

$$b = \frac{\dot{m}_{wet\ air}}{\dot{m}_{diesel}} \frac{M_{diesel}}{M_{wet\ air}} = A/F\Big|_{wet} \frac{M_{diesel}}{M_{wet\ air}}$$