TRP LABORATORIES

CyFlex® Knowledge Article

Burned Gas Composition from Measured Concentration

Author: Daniel Oren

July 9, 2019

Background

The *Burned Gas Composition* document describes a simple method for calculating the burned gas composition assuming that the composition and mass flow rates of the component gas are known using the reaction equation:

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

where

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

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

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

In this document we describe a method for calculating the mass flow rate of one of the component streams assuming lean combustion and given the mass flow rate of the remaining component streams, the stream compositions and the measured concentration of either oxygen or carbon dioxide in the burned gas.

Atom Balances

The atom balance equations bgc.3 - bgc.8 need to be rewritten in a slightly different form to isolate the molar flow rates:

C:

$$\boxed{\begin{aligned} & \left.\begin{matrix} a\left(w_{C,A}\, y_{A,a} + w_{C,B}\, y_{B,a} + w_{C,C}\, y_{C,a} + \ldots\right) + \\ b\left(w_{C,A}\, y_{A,b} + w_{C,B}\, y_{B,b} + w_{C,C}\, y_{C,b} + \ldots\right) + \\ \ldots \end{matrix}\right\} \;=\; \Pi \\ & = \; a(\Pi_a) + b(\Pi_b) + c(\Pi_c) + \ldots \\ & = \; \beta \; + \; \delta \end{aligned}} \qquad \text{bf.2}$$

H:

$$\boxed{\begin{aligned} & \left.\begin{matrix} a\left(w_{H,A}\, y_{A,a} + w_{H,B}\, y_{B,a} + w_{H,C}\, y_{C,a} + \ldots\right) + \\ b\left(w_{H,A}\, y_{A,b} + w_{H,B}\, y_{B,b} + w_{H,C}\, y_{C,b} + \ldots\right) + \\ \ldots \end{matrix}\right\} \;=\; \Theta \\ & = \; a(\Theta_a) + b(\Theta_b) + c(\Theta_c) + \ldots \\ & = \; 2\alpha + 2\eta \end{aligned}} \qquad \text{bf.3}$$

O:

$$\left.\begin{array}{l} a\left(w_{O,A}\, y_{A,a} + w_{O,B}\, y_{B,a} + w_{O,C}\, y_{C,a} + \ldots\right)+ \\ b\left(w_{O,A}\, y_{A,b} + w_{O,B}\, y_{B,b} + w_{O,C}\, y_{C,b} + \ldots\right)+ \\ \ldots \end{array}\right\} = \Sigma$$

$$= a\left(\Sigma_a\right)+b\left(\Sigma_b\right)+c\left(\Sigma_c\right)+\ldots$$

$$= \alpha + 2\beta + 2\gamma + \delta \qquad \text{bf.4}$$

N:

$$\left.\begin{array}{l} a\left(w_{N,A}\, y_{A,a} + w_{N,B}\, y_{B,a} + w_{N,C}\, y_{C,a} + \ldots\right)+ \\ b\left(w_{N,A}\, y_{A,b} + w_{N,B}\, y_{B,b} + w_{N,C}\, y_{C,b} + \ldots\right)+ \\ \ldots \end{array}\right\} = \Delta$$

$$= a\left(\Delta_a\right)+b\left(\Delta_b\right)+c\left(\Delta_c\right)+\ldots$$

$$= 2\lambda \qquad \text{bf.5}$$

A:

$$\left.\begin{array}{l} a\left(w_{A,A}\, y_{A,a} + w_{A,B}\, y_{B,a} + w_{A,C}\, y_{C,a} + \ldots\right)+ \\ b\left(w_{A,A}\, y_{A,b} + w_{A,B}\, y_{B,b} + w_{A,C}\, y_{C,b} + \ldots\right)+ \\ \ldots \end{array}\right\} = \Omega$$

$$= a\left(\Omega_a\right)+b\left(\Omega_b\right)+c\left(\Omega_c\right)+\ldots$$

$$= \psi \qquad \text{bf.6}$$

S:

$$\left.\begin{array}{l} a\left(w_{S,A}\, y_{A,a} + w_{S,B}\, y_{B,a} + w_{S,C}\, y_{C,a} + \ldots\right)+ \\ b\left(w_{S,A}\, y_{A,b} + w_{S,B}\, y_{B,b} + w_{S,C}\, y_{C,b} + \ldots\right)+ \\ \ldots \end{array}\right\} = \Lambda$$

$$= a\left(\Lambda_a\right)+b\left(\Lambda_b\right)+c\left(\Lambda_c\right)+\ldots$$

$$= \omega \qquad \text{bf.7}$$

where:

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

Measured Exhaust Gas Concentration

The measured exhaust gas concentration of carbon dioxide or oxygen can be related to the burned gas composition through bgc.42 and bgc.43 reproduced here as bf.8 and bf.9 respectively.

$$y_{CO_2,burned,dry} = \frac{\beta}{\beta+\gamma+\delta+\eta+\lambda+\psi+\omega} \qquad \text{bf.8}$$

$$y_{O_2,burned,dry} = \frac{\gamma}{\beta+\gamma+\delta+\eta+\lambda+\psi+\omega} \qquad \text{bf.9}$$

For stoichiometric or lean mixtures, we know that:

$$\delta = 0 \quad and \quad \eta = 0 \qquad \text{bf.10}$$

And:

$$\beta = \Pi \qquad \text{bf.11}$$

$$\alpha = \frac{\Theta}{2} \qquad \text{bf.12}$$

$$\gamma = \frac{\Sigma - \alpha - 2\beta}{2} = \frac{\Sigma}{2} - \frac{\Theta}{4} - \Pi \qquad \text{bf.13}$$

$$\lambda = \frac{\Delta}{2} \qquad \text{bf.14}$$

$$\psi = \Omega \qquad \text{bf.15}$$

$$\omega = \Lambda \qquad \text{bf.16}$$

Substituting bf.10 through bf.16 into bf.8 gives:

$$\begin{aligned} y_{CO_2,burned,dry} &= \frac{\Pi}{\Pi+\frac{\Sigma}{2}-\frac{\Theta}{4}-\Pi+\frac{\Delta}{2}+\Omega+\Lambda} \\ &= \frac{\Pi}{\frac{\Sigma}{2}-\frac{\Theta}{4}+\frac{\Delta}{2}+\Omega+\Lambda} \end{aligned} \qquad \text{bf.17}$$

For the purposes of this discussion, we will assume that we don't know the mass flow rate of stream *a*. Using the recast atom balance equations to isolate each stream gives:

$$y_{CO_2,burned,dry} = \frac{a(\Pi_a)+b(\Pi_b)+c(\Pi_c)+\ldots}{\left\{\begin{array}{l} a\left(\frac{\Sigma_a}{2}-\frac{\Theta_a}{4}+\frac{\Delta_a}{2}+\Omega_a+\Lambda_a\right)+b\left(\frac{\Sigma_b}{2}-\frac{\Theta_b}{4}+\frac{\Delta_b}{2}+\Omega_b+\Lambda_b\right)+ \\ c\left(\frac{\Sigma_c}{2}-\frac{\Theta_c}{4}+\frac{\Delta_c}{2}+\Omega_c+\Lambda_c\right)+\ldots \end{array}\right\}} \qquad \text{bf.18}$$

Since we know the component stream compositions, the measured dry concentration of carbon dioxide in the burned gas and all the mole flow rates except *a*, we can rearrange the equation to solve for *a*:

$$a = \frac{\left\{ \begin{array}{l} b\left(\Pi_b\right) + c\left(\Pi_c\right) + \ldots - y_{CO_2,burned,dry}\left[b\left(\frac{\Sigma_b}{2} - \frac{\Theta_b}{4} + \frac{\Delta_b}{2} + \Omega_b + \Lambda_b\right) + \right. \\ \left. c\left(\frac{\Sigma_c}{2} - \frac{\Theta_c}{4} + \frac{\Delta_c}{2} + \Omega_c + \Lambda_c\right) + \ldots \right] \end{array} \right\}}{y_{CO_2,burned,dry}\left(\frac{\Sigma_a}{2} - \frac{\Theta_a}{4} + \frac{\Delta_a}{2} + \Omega_a + \Lambda_a\right) - \left(\Pi_a\right)} \qquad \text{bf.19}$$

A similar development can be used if we start with the measured burned gas oxygen concentration and bf.9

$$y_{O_2,burned,dry} = \frac{\frac{\Sigma}{2} - \frac{\Theta}{4} - \Pi}{\frac{\Sigma}{2} - \frac{\Theta}{4} + \frac{\Delta}{2} + \Omega + \Lambda} \qquad \text{bf.20}$$

$$a = \frac{\left\{ \begin{array}{l} b\left(\frac{\Sigma_b}{2} - \frac{\Theta_b}{4} - \Pi_b\right) + c\left(\frac{\Sigma_c}{2} - \frac{\Theta_c}{4} - \Pi_c\right) + \ldots - y_{O_2,burned,dry} \times \\ \left[b\left(\frac{\Sigma_b}{2} - \frac{\Theta_b}{4} + \frac{\Delta_b}{2} + \Omega_b + \Lambda_b\right) + c\left(\frac{\Sigma_c}{2} - \frac{\Theta_c}{4} + \frac{\Delta_c}{2} + \Omega_c + \Lambda_c\right) + \ldots \right] \end{array} \right\}}{y_{O_2,burned,dry}\left(\frac{\Sigma_a}{2} - \frac{\Theta_a}{4} + \frac{\Delta_a}{2} + \Omega_a + \Lambda_a\right) - \left(\frac{\Sigma_a}{2} - \frac{\Theta_a}{4} - \Pi_a\right)} \qquad \text{bf.21}$$

Carbon dioxide and oxygen are species that are routinely measured in the exhaust gas. Water vapor concentration is seldom measured, but a calculation based on a given water vapor concentration is still quite valuable for analyzing situations where condensation might occur, e.g. in an EGR cooler or an exhaust aftertreatment device. The burned gas water vapor concentration is given by bgc.32 which is reproduced here as bf.22.

$$y_{H_2O,burned,wet} = \frac{\alpha}{\alpha + \beta + \gamma + \delta + \eta + \lambda + \psi + \omega} \qquad \text{bf.22}$$

Note that the denominator is different than in the equations for oxygen and carbon dioxide since the measured or assumed value is made on a wet basis. Substituting bf.10 through bf.16 int bf.22 gives:

$$y_{H_2O,burned,wet} = \frac{\frac{\Theta}{2}}{\frac{\Theta}{2}+\Pi+\frac{\Sigma}{2}-\frac{\Theta}{4}-\Pi+\frac{\Delta}{2}+\Omega+\Lambda} = \frac{\frac{\Theta}{2}}{\frac{\Sigma}{2}+\frac{\Theta}{4}+\frac{\Delta}{2}+\Omega+\Lambda} \qquad \text{bf.23}$$

Using the same method as before and solving for *a* gives:

$$a = \frac{\left\{ b\left(\frac{\Theta_b}{2}\right)+c\left(\frac{\Theta_c}{2}\right)+\ldots - y_{H_2O,burned,wet}\left[b\left(\frac{\Sigma_b}{2}+\frac{\Theta_b}{4}+\frac{\Delta_b}{2}+\Omega_b+\Lambda_b\right)+ c\left(\frac{\Sigma_c}{2}+\frac{\Theta_c}{4}+\frac{\Delta_c}{2}+\Omega_c+\Lambda_c\right)+\ldots\right]\right\}}{y_{H_2O,burned,wet}\left(\frac{\Sigma_a}{2}+\frac{\Theta_a}{4}+\frac{\Delta_a}{2}+\Omega_a+\Lambda_a\right)-\left(\frac{\Theta_a}{2}\right)} \qquad \text{bf.24}$$

The mass flow rate of stream *a* can now be computed using:

$$\dot{m}_a = a\,M_a \qquad \text{bf.23}$$

We now have all the necessary inputs for the standard burned gas composition calculation.