A Reference Guide for Specifying Combustion Chemistry Ratios in the CFAST and FASTLite Zone Models

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Introduction

A method is presented for calculating the appropriate ratios required by the combustion chemistry model implemented in CFAST and FASTLite. The procedure has been developed for hydrocarbon fuels of a known chemical composition (which may include Oxygen and/or Nitrogen) in conjunction with values for the yield of Carbon Dioxide, Carbon Monoxide, and Soot per unit mass of fuel consumed. A methodology has been developed for calculating the combustion chemistry ratios and is illustrated with a specific example.

CFAST Requirements

The combustion ratios required by CFAST are on a mass basis and shown in Table 1 below.

Ratio	***Definition***	***Line in .DAT file***
H/C	Mass of Hydrogen to mass of Carbon in fuel composition	HCR
O/C	Mass of Oxygen to mass of Carbon in fuel composition	O2
HCN	Mass of Hydrogen Cyanide products per unit mass of fuel consumed	HCN
HCL	Mass of Hydrogen Chloride products per unit mass of fuel consumed	HCL
C/CO2	Mass of Carbon products per unit mass of Carbon Dioxide products	OD
CO/CO2	Mass of Carbon Monoxide per unit mass of Carbon Dioxide in products	CO

Table 1 -- Ratios used in the CFAST/FASTLite combustion chemistry model.

While the first two ratios H/C and O/C can be readily determined from the fuel composition alone, the remaining ratios require knowledge of the combustion reaction of the fuel.

Input Variables

The inputs required for properly applying this method of calculating the CFAST combustion ratios are detailed below in Table 2.

Input	***Description***
$C_aH_bO_cN_d$	Chemical composition of fuel which can contain Carbon, Hydrogen, Oxygen, and Nitrogen
Y_{CO2}	Mass of Carbon Dioxide produced per unit mass of fuel consumed
Y_{CO}	Mass of Carbon Monoxide produced per unit mass of fuel consumed
Y_s	Mass of Carbon (soot) produced per unit mass of fuel consumed

Table 2 -- Input variables required to calculate the combustion chemistry ratios.

Chemical Balance of Combustion Reaction

A general combustion equation for the oxidation of a fuel that contains Carbon, Hydrogen, Oxygen, and Nitrogen is given in Equation (1). The reaction is assumed to produce Carbon Dioxide, Water Vapor, Carbon Monoxide, Hydrogen Cyanide, Soot (assumed to be elemental Carbon), and excess inert Nitrogen.

$$C_aH_bO_cN_d + e(O_2 + 3.76N_2) \rightarrow fCO_2 + gH_2O + hCO + iHCN + jC + kN_2 \qquad (1)$$

The number of moles of Carbon, Hydrogen, Oxygen, and Nitrogen are separated into algebraic expressions based on the above chemical reaction.

$$C: \quad a = f + h + i + j \qquad (2)$$

$$H: \quad b = 2g + i \qquad (3)$$

$$O: \quad c + 2e = 2f + g + h \qquad (4)$$

$$N: \quad d + 7.52e = i + 2k \qquad (5)$$

Seven variables are known in the algebraic expressions shown above in Equations (2) through (5) and appear in Table 3 below.

Variable	***Known From***
a	Carbon moles in fuel composition
b	Hydrogen moles in fuel composition
c	Oxygen moles in fuel composition
d	Nitrogen moles in fuel composition
f	Carbon dioxide moles in products, derived from Y_{CO2}
h	Carbon monoxide moles in products, derived from Y_{CO}
j	Soot moles in products, derived from Y_s

Table 3 -- Known variables in balanced equation of combustion reaction.

Therefore, four variables are unknown and are shown in the Table 4 below.

Variable	***Representing***
e	Moles of air necessary for stoichiometric combustion
g	Moles of Water Vapor in products
i	Moles of Hydrogen Cyanide in products
k	Moles of excess inert Nitrogen

Table 4 -- Unknown variables from balanced equation of combustion reaction.

The four unknowns (*e*, *g*, *i*, *k*) are part of the four algebraic equations, which can be solved simultaneously. Equation (2) contains only one unknown, *i*, and can be rearranged for in terms of the other known quantities.

$$i = a - f - h - j \qquad (6)$$

Equation (3) can then be solved for the unknown value of *g* using the result of (6).

$$g = \frac{b - i}{2} \qquad (7)$$

The result of Equation (7) can then be applied, with other known variables, to compute *e* from (4) in the following manner.

$$e = \frac{2f + g + h - c}{2} \qquad (8)$$

The unknown variable *k* can be calculated using known values in Equation (5).

$$k = \frac{d + 7.52e - i}{2} \qquad (9)$$

The results of Equations (6) through (9) are rearranged into a format more suitable for general use with the inclusion of mole numbers.

$$n_{HCN(products)} = n_{C(fuel)} - n_{CO_2(products)} - n_{CO(products)} - n_{C(products)} \qquad (10)$$

$$n_{H_2O(products)} = \frac{n_{H(fuel)} - n_{HCN(products)}}{2} \qquad (11)$$

$$n_{Air(oxidant)} = \frac{2n_{CO_2(products)} + n_{H_2O(products)} + n_{CO(products)} - n_{O(fuel)}}{2} \qquad (12)$$

$$n_{N_2(products)} = \frac{n_{N(fuel)} + 7.52n_{Air(oxidant)} - n_{HCN(products)}}{2} \qquad (13)$$

After computing the mole numbers of the variables above, the combustion ratios required by CFAST can be calculated.

Examples of Determining CFAST Combustion Ratios

A sample calculation of CFAST combustion ratios is provided to illustrate a general methodology that could be adopted for routine use. The example relies upon data from the literature, specifically “Generation of Heat and Chemical Compounds in Fires” by Tewarson in Section 3 Chapter 4 of the *SFPE Handbook of Fire Protection Engineering* 2^{nd} *Edition*, 1995. Experimental data from the Room Calorimeter, for example, can also be used in the context of this methodology.

Consider the combustion of the flexible polyurethane foam GM 21. The chemical composition of the fuel is given in Table 3-4.10 of Tewarson as,

$CH_{1.8}O_{0.30}N_{0.05}$

The yields of Carbon Dioxide, Carbon Monoxide, and Carbon (soot) for GM 21 are reported in Table 3-4.11 of Tewarson as,

$y_{CO2} = 1.55$
$y_{CO} = 0.010$
$y_s = 0.131$

The above yields are a mass of product per unit mass of fuel and need to be expressed on a molar basis. The general form of this conversion begins with the definition of the product yield,

$$y_{product} = \frac{m_{product}}{m_{fuel}} = \frac{n_{product} MW_{product}}{n_{fuel} MW_{fuel}} \qquad (14)$$

where,

m_i – mass of product i
n_i – moles of product i
MW_i – molecular weight of product i

The moles of fuel are defined as unity to be consistent with the balanced equation of the combustion reaction. Therefore, the number of moles of general product is related to the product yield in the following manner,

$$n_{product} = y_{product}\left(\frac{MW_{fuel}}{MW_{product}}\right) \qquad (15)$$

The expression above can be applied to compute the number of moles of Carbon Dioxide, Carbon Monoxide, and Carbon (soot) on the product side of the combustion reaction.

The molecular weight of the fuel is,

$$MW_{fuel} = (1\cdot 12) + (1.8\cdot 1) + (0.30\cdot 16) + (0.05\cdot 14) = 19.3$$

The molecular weights of the three products are,

$$MW_{CO_2} = (1\cdot 12) + (2\cdot 16) = 44$$
$$MW_{CO} = (1\cdot 12) + (1\cdot 16) = 28$$
$$MW_{soot} = (1\cdot 12) = 12$$

The number of moles for the three products are,

$$n_{CO_2} = y_{CO_2}\left(\frac{MW_{fuel}}{MW_{CO_2}}\right) = 1.55\left(\frac{19.3}{44}\right) = 0.68$$

$$n_{CO} = y_{CO}\left(\frac{MW_{fuel}}{MW_{CO}}\right) = 0.010\left(\frac{19.3}{28}\right) = 0.0069$$

$$n_{C} = y_{C}\left(\frac{MW_{fuel}}{MW_{C}}\right) = 0.131\left(\frac{19.3}{12}\right) = 0.21$$

Equations (10) through (13) can now be solved using the results from above in conjunction with the number of moles of elements in the fuel.

$$n_{HCN(products)} = n_{C(fuel)} - n_{CO_2(products)} - n_{CO(products)} - n_{C(products)}$$

$$n_{HCN(products)} = 1 - 0.68 - 0.0069 - 0.21 = 0.1031$$

$$n_{H_2O(products)} = \frac{n_{H(fuel)} - n_{HCN(products)}}{2}$$

$$n_{H_2O(products)} = \frac{1.8 - 0.1031}{2} = 0.8484$$

$$n_{Air(oxidant)} = \frac{2n_{CO_2(products)} + n_{H_2O(products)} + n_{CO(products)} - n_{O(fuel)}}{2}$$

$$n_{Air(oxidant)} = \frac{2 \cdot 0.68 + 0.8484 + 0.0069 - 0.30}{2} = 0.9576$$

$$n_{N_2(products)} = \frac{n_{N(fuel)} + 7.52 n_{Air(oxidant)} - n_{HCN(products)}}{2}$$

$$n_{N_2(products)} = \frac{0.05 + 7.52 \cdot 0.9576 - 0.1031}{2} = 3.5740$$

The combustion chemistry ratios can be calculated using the known values computed above.

$$H/C = \frac{n_{H(fuel)} MW_H}{n_{C(fuel)} MW_C} = \frac{(1.8)(1)}{(1)(12)} = 0.15$$

$$O/C = \frac{n_{O(fuel)} MW_O}{n_{C(fuel)} MW_C} = \frac{(0.30)(16)}{(1)(12)} = 0.40$$

$$HCN/Fuel = \frac{n_{HCN\,(products)} MW_{HCN}}{n_{Fuel} MW_{Fuel}} = \frac{(0.1031)(27)}{(1)(19.3)} = 0.144$$

$$C/CO_2 = \frac{n_{C\,(products)} MW_{C}}{n_{CO_2\,(products)} MW_{CO_2}} = \frac{(0.21)(12)}{(0.68)(44)} = 0.084$$

$$CO/CO_2 = \frac{n_{CO\,(products)} MW_{CO}}{n_{CO_2\,(products)} MW_{CO_2}} = \frac{(0.0069)(28)}{(0.68)(44)} = 0.0064$$