Given Products, Calculate Fuel using "Simple" Chemistry Model in FDS

For the simple chemistry model in FDS, each reaction is assumed to be of the form:

$$C_xH_yO_zN_v + \nu_{O_2}O_2 \xrightarrow{yields} \nu_{CO_2}CO_2 + \nu_{H_2O}H_2O + \nu_{CO}CO + \nu_S Soot + \nu_{N_2}N_2 \tag{1}$$

where:

ν_j is stoichiometric coefficient of product j
W_j is mass of component j
Y_j is yield of product j (mass generation rate of product j/total mass loss rate)

However, there are times when we are given combustion products, but not the corresponding fuel composition. If we know the *yields* of all of the products we can solve for a corresponding fuel composition and required oxygen that will correspond to the yields.

For the simple chemistry model in FDS, knowing products means that we know the yields (Y_{CO_2}, Y_{H_2O}, Y_{CO}, Y_S, and Y_{N_2}) and that we know the fraction of the atoms in the soot that are hydrogen (X_H). In this case, the unknowns are the fuel composition (x, y, z, v) and the stoichiometric coefficient of oxygen (ν_{O_2}). We will address the case of incomplete product knowledge later.

The yields are given as the mass of product per unit fuel mass. We can convert between yields and stoichiometric coefficients (moles) using the molecular mass. For component j:

$$\nu_j = \frac{W_{Fuel}}{W_j} Y_j \tag{2}$$

Unfortunately, we do not yet know the composition of the fuel, so must write it using the unknown values.

$$W_F = xW_C + yW_H + zW_O + \mathrm{v}W_N \tag{3}$$

We proceed to evaluate each stoichiometric coefficient:

$$\nu_{CO2} = \frac{W_F}{W_{CO2}} Y_{CO2}$$

$$\nu_{CO2} = \frac{(xW_C + yW_H + zW_O + \mathrm{v}W_N)}{W_{CO2}} Y_{CO2}$$

$$\nu_{CO2} = (xW_C + yW_H + zW_O + vW_N)\left(\frac{Y_{CO2}}{W_{CO2}}\right) \tag{4}$$

In exactly the same pattern, we can write the other stoichiometric coefficients:

$$\nu_{H2O} = (xW_C + yW_H + zW_O + vW_N)\left(\frac{Y_{H2O}}{W_{H2O}}\right) \tag{5}$$

$$\nu_S = (xW_C + yW_H + zW_O + vW_N)\left(\frac{Y_S}{W_S}\right) \tag{6}$$

$$\nu_{CO} = (xW_C + yW_H + zW_O + vW_N)\left(\frac{Y_{CO}}{W_{CO}}\right) \tag{7}$$

$$v_{N2} = (xW_C + yW_H + zW_O + vW_N)\left(\frac{Y_{N2}}{W_{N2}}\right) \quad (8)$$

Soot is assumed to be composed of carbon and hydrogen:

$$Soot = X_H H + (1 - X_H)C \quad (9)$$

so the molecular mass of the soot is given by:

$$W_S = X_H W_H + (1 - X_H)W_C \quad (10)$$

Atomic balances for C, H, O, and N give us four equations we can put in matrix form.

The components that contain carbon (C) are $Fuel$, CO_2, CO, and $Soot$. Performing an atomic balance for C gives:

$$x - \left[(xW_C + yW_H + zW_O + vW_N)\left(\frac{Y_{CO2}}{W_{CO2}}\right)\right]$$
$$- \left[(xW_C + yW_H + zW_O + vW_N)\left(\frac{Y_{CO}}{W_{CO}}\right)\right]$$
$$- \left[(xW_C + yW_H + zW_O + vW_N)\left(\frac{(1 - X_H)Y_S}{W_S}\right)\right] = 0$$

Collecting terms:

$$x\left[1 - W_C\left(\frac{Y_{CO2}}{W_{CO2}} + \frac{Y_{CO}}{W_{CO}} + \frac{(1 - X_H)Y_S}{W_S}\right)\right]$$
$$- y\left[W_H\left(\frac{Y_{CO2}}{W_{CO2}} + \frac{Y_{CO}}{W_{CO}} + \frac{(1 - X_H)Y_S}{W_S}\right)\right]$$
$$- z\left[W_O\left(\frac{Y_{CO2}}{W_{CO2}} + \frac{Y_{CO}}{W_{CO}} + \frac{(1 - X_H)Y_S}{W_S}\right)\right]$$
$$- v\left[W_N\left(\frac{Y_{CO2}}{W_{CO2}} + \frac{Y_{CO}}{W_{CO}} + \frac{(1 - X_H)Y_S}{W_S}\right)\right] = 0$$

If we define a constant $A1$:

$$A1 = \left(\frac{Y_{CO2}}{W_{CO2}} + \frac{Y_{CO}}{W_{CO}} + \frac{(1-X_H)Y_S}{W_S}\right) \quad (11)$$

this simplifies to:

$$x[1 - W_C(A1)] - y[W_H(A1)] - z[W_O(A1)] - v[W_N(A1)] = 0 \quad (12)$$

which provides the first row of our solution matrix.

Proceeding in exactly the same manner for hydrogen:

$$A2 = \left(2\frac{Y_{H2O}}{W_{H2O}} + \frac{X_H Y_S}{W_S}\right) \quad (13)$$

$$-x[W_C(A2)] + y[1 - W_H(A2)] - z[W_O(A2)] - v[W_N(A2)] = 0 \quad (14)$$

For oxygen:

$$A3 = \left(2\frac{Y_{CO2}}{W_{CO2}} + \frac{Y_{H2O}}{W_{H2O}} + \frac{Y_{CO}}{W_{CO}}\right) \tag{15}$$

$$-x[W_C(A3)] - y[W_H(A3)] + z[1 + W_O(A3)] - v[W_N(A3)] = 0 \tag{16}$$

For nitrogen:

$$A4 = \left(2\frac{Y_{N2}}{W_{N2}}\right) \tag{17}$$

$$-x[W_C(A4)] - y[W_H(A4)] - z[W_O(A4)] + v[1 - W_N(A4)] = 0 \tag{18}$$

We now have four equations, but we have five unknowns. When specifying the fuel composition, we are free to define one of the values and the others will be scaled relative. Our last equation then is:

$$x = 1 \tag{19}$$

We can now assemble our matrix and solve for the unknowns:

$$\begin{bmatrix} (1 - W_C A1) & (W_H A1) & (W_O A1) & (W_N A1) & 0 \\ (W_C A2) & (1 - W_H A2) & (W_O A2) & (W_N A2) & 0 \\ (W_C A3) & (W_H A3) & (1 - W_O A3) & (W_N A3) & 0 \\ (W_C A4) & (W_H A4) & (W_O A4) & (1 - W_N A4) & 0 \\ 1 & 0 & 0 & 0 & 0 \end{bmatrix} \begin{Bmatrix} x \\ y \\ z \\ v \\ v_{O_2} \end{Bmatrix} = \begin{Bmatrix} 0 \\ 0 \\ 0 \\ 0 \\ 1 \end{Bmatrix} \tag{20}$$