PART 1 - B

Equations

function $getenthalpy(S\$,\ T)$ (1)

This function uses the NASA external procedure to return the enthalpy of reactant species S$ at T.

call $NASA(S\$,\ T : cp,\ geTenthalpy,\ s)$ (2)

end $getenthalpy$ (3)

procedure $enthalpygibbs(S\$,\ T : h,\ g)$ (4)

This procedure uses the NASA external procedure to return the enthalpy and Gibbs energy of product species S$ at T.

call $NASA(S\$,\ T : cp,\ h,\ s)$ (5)

$g := h - T \cdot s$ (6)

end h_g (7)

Reaction: 0.9 CH4 + 0.1 C2H6 + a (O2 + 3.76 N2) $\longleftarrow\!\!\longrightarrow$ b CO2 + c H2O + d N2 + e O2 + f O + g N + j H + k OH + m H2 + n CO + >>>p CH4 + q C2H6<<<

$T_{air} = 460\ \text{[K]}$ (8)

$T_{fuel} = 430\ \text{[K]}$ (9)

$T_{final,1} = 1700\ \text{[K]}$ (10)

$T_{final,2} = 1600\ \text{[K]}$ (11)

$T_{final,3} = 1300\ \text{[K]}$ (12)

$P = 1000\ \text{[kPa]}$ (13)

$P_{ref} = 100\ \text{[kPa]}$ (14)

$R = R\#$ Universal gas constant (15)

$h_{N2,inlet} = getenthalpy(\text{'N2'},\ T_{air})$ (16)

$h_{O2,inlet} = getenthalpy(\text{'O2'},\ T_{air})$ (17)

$h_{CH4,inlet} = getenthalpy(\text{'CH4'},\ T_{fuel})$ (18)

$h_{C2H6,inlet} = getenthalpy(\text{'C2H6'},\ T_{fuel})$ (19)

$h_{fuel,inlet} = 0.9 \cdot h_{CH4,inlet} + 0.1 \cdot h_{C2H6,inlet}$ (20)

duplicate $i = 1,\ 3$ (21)

Stoichiometry for a basis of 1 kmol of fuel

$1.1 = b_i + n_i$ Carbon balance (22)

$$4.2 = 2 \cdot c_i + j_i + k_i + 2 \cdot m_i \quad \text{Hydrogen balance} \tag{23}$$

$$2 \cdot a_i = 2 \cdot b_i + c_i + 2 \cdot e_i + f_i + k_i + n_i \quad \text{Oxygen balance} \tag{24}$$

$$3.76 \cdot 2 \cdot a_i = 2 \cdot d_i + g_i \quad \text{Nitrogen balance} \tag{25}$$

Total moles of gas and mole fractions.

$$n_{tot,i} = (b_i + c_i + d_i + e_i + f_i + g_i + j_i + k_i + m_i + n_i) \tag{26}$$

$$y_{CO2,i} \cdot n_{tot,i} = b_i \tag{27}$$

$$y_{H2O,i} \cdot n_{tot,i} = c_i \tag{28}$$

$$y_{N2,i} \cdot n_{tot,i} = d_i \tag{29}$$

$$y_{O2,i} \cdot n_{tot,i} = e_i \tag{30}$$

$$y_{O,i} \cdot n_{tot,i} = f_i \tag{31}$$

$$y_{N,i} \cdot n_{tot,i} = g_i \tag{32}$$

$$y_{H,i} \cdot n_{tot,i} = j_i \tag{33}$$

$$y_{OH,i} \cdot n_{tot,i} = k_i \tag{34}$$

$$y_{H2,i} \cdot n_{tot,i} = m_i \tag{35}$$

$$y_{CO,i} \cdot n_{tot,i} = n_i \tag{36}$$

The following equations provide the enthalpy for each chemical species at the inlet tempretures and T_{final} and the reference pressure of 10 bar. The NASA external procedure is used in the Function getenthalpy to calculate h at the equilibrium temperature, which is determined from an energy balance.

$$\text{call } enthalpygibbs(\text{`CO2'}, T_{final,i} : h_{CO2,i}, g^o_{CO2,i}) \tag{37}$$

$$\text{call } enthalpygibbs(\text{`H2O'}, T_{final,i} : h_{H2O,i}, g^o_{H2O,i}) \tag{38}$$

$$\text{call } enthalpygibbs(\text{`N2'}, T_{final,i} : h_{N2,i}, g^o_{N2,i}) \tag{39}$$

$$\text{call } enthalpygibbs(\text{`O2'}, T_{final,i} : h_{O2,i}, g^o_{O2,i}) \tag{40}$$

$$\text{call } enthalpygibbs(\text{`O'}, T_{final,i} : h_{O,i}, g^o_{O,i}) \tag{41}$$

$$\text{call } enthalpygibbs(\text{`N'}, T_{final,i} : h_{N,i}, g^o_{N,i}) \tag{42}$$

$$\text{call } enthalpygibbs(\text{`H'}, T_{final,i} : h_{H,i}, g^o_{H,i}) \tag{43}$$

$$\text{call } enthalpygibbs(\text{`OH'}, T_{final,i} : h_{OH,i}, g^o_{OH,i}) \tag{44}$$

$$\text{call } enthalpygibbs(\text{`H2'}, T_{final,i} : h_{H2,i}, g^o_{H2,i}) \tag{45}$$

$$\text{call } enthalpygibbs(\text{`CO'}, T_{final,i} : h_{CO,i}, g^o_{CO,i}) \tag{46}$$

Call EnthalpyGibbs('CH4',$T_{final,i}$: $h_{CH4,i}$, $g^o{}_{CH4,i}$)
Call EnthalpyGibbs('C2H6',$T_{final,i}$: $h_{C2H6,i}$, $g^o{}_{C2H6,i}$)
$h_{fuel,i}$ = 0.9 * $h_{CH4,i}$ + 0.1 * $h_{C2H6,i}$
$g^o{}_{fuel,i}$ = 0.9 * $g^o{}_{CH4,i}$ + 0.1 * $g^o{}_{C2H6,i}$

Standard-state Gibbs Free Energy change for our 6 reactions.

This block of code was replaced with the manual calculation of the equilibrium constants present at appendix A of this file. I have no Idea why this segment didnt work, especially seeing that it performed just fine for the first and third segments and just had trouble calculating part 2 (it gave me the rich value of the AF ratio corresponding to 1600 [K] final temprature, one that claimed a[2] = 1.008 and $\dot{m}_2 < 0$), but since I didnt have time to troubleshoot it propardly, I just used the brute force method of calculating with pen and paper

$\Delta G^o{}_{1,i}$ = (2 * g$^o{}_{N,i}$) - g$^o{}_{N2,i}$
DELTAG$^o{}_{2,i}$ = (2 * g$^o{}_{O,i}$) - g$^o{}_{O2,i}$
DELTAG$^o{}_{3,i}$ = (2 * g$^o{}_{H,i}$) - g$^o{}_{H2,i}$
DELTAG$^o{}_{4,i}$ = (2 * g$^o{}_{OH,i}$) - g$^o{}_{O2,i}$ - g$^o{}_{H2,i}$
DELTAG$^o{}_{5,i}$ = (2 * g$^o{}_{CO2,i}$) - g$^o{}_{O2,i}$ - (2 * g$^o{}_{CO,i}$)
DELTAG$^o{}_{6,i}$ = (4 * g$^o{}_{OH,i}$) - g$^o{}_{O2,i}$ - (2 * g$^o{}_{H2O,i}$)

Law of Mass Action for reactions 1 through 6

This block of code was replaced with the manual calculation of the equilibrium constants present at appendix A of this file. I have no Idea why this segment didnt work, especially seeing that it performed just fine for the first and third segments and just had trouble calculating part 2 (it gave me the rich value of the AF ratio corresponding to 1600 [K] final temprature, one that claimed a[2] = 1.008 and $\dot{m}_2 < 0$), but since I didnt have time to troubleshoot it propardly, I just used the brute force method of calculating with pen and paper

$\Delta G^o{}_{1,i}$ = -1 * R * T$_{final,i}$ * ln(K$_{1,i}$)
DELTAG$^o{}_{2,i}$ = -1 * R * T$_{final,i}$ * ln(K$_{2,i}$)
DELTAG$^o{}_{3,i}$ = -1 * R * T$_{final,i}$ * ln(K$_{3,i}$)
DELTAG$^o{}_{4,i}$ = -1 * R * T$_{final,i}$ * ln(K$_{4,i}$)
DELTAG$^o{}_{5,i}$ = -1 * R * T$_{final,i}$ * ln(K$_{5,i}$)
DELTAG$^o{}_{6,i}$ = -1 * R * T$_{final,i}$ * ln(K$_{6,i}$)

Definition of equilibrium constant for reactions 1 through 6

$$K_{1,i} \cdot y_{N2,i} = \left(y^2_{N,i}\right) \cdot (P/P_{ref}) \tag{47}$$

$$K_{2,i} \cdot y_{O2,i} = \left(y^2_{O,i}\right) \cdot (P/P_{ref}) \tag{48}$$

$$K_{3,i} \cdot y_{H2,i} = \left(y^2_{H,i}\right) \cdot (P/P_{ref}) \tag{49}$$

$$K_{4,i} \cdot y_{O2,i} \cdot y_{H2,i} = \left(y^2_{OH,i}\right) \tag{50}$$

$$K_{5,i} \cdot y_{O2,i} \cdot \left(y^2_{CO,i}\right) \cdot (P/P_{ref}) = \left(y^2_{CO2,i}\right) \tag{51}$$

$$K_{6,i} \cdot y_{O2,i} \cdot \left(y^2_{H2O,i}\right) = \left(y^4_{OH,i}\right) \cdot (P/P_{ref}) \tag{52}$$

Find the enthalpy of the reactants

$$HR_i = h_{fuel,inlet} + a_i \cdot h_{O2,inlet} + 3.76 \cdot a_i \cdot h_{N2,inlet} \tag{53}$$

Find the enthalpy of products

$$HP_i = (b_i \cdot h_{CO2,i}) + (c_i \cdot h_{H2O,i}) + (d_i \cdot h_{N2,i}) + (e_i \cdot h_{O2,i}) + (f_i \cdot h_{O,i}) + (g_i \cdot h_{N,i}) + (j_i \cdot h_{H,i}) + (k_i \cdot h_{OH,i}) + (m_i \cdot h_{H2,i}) + (n_i \cdot h$$

Apply an adiabatic energy balance to determine the product temperature

$$HR_i = HP_i \tag{55}$$

end (56)

1 kmol of fuel weighs the same as 0.9 kmol of CH4 and 0.1 kmol of C2H6, = 0.9 * 16.043 + 0.1 * 30.07 = 17.4457 kg/kmol, so 0.07 kg/s fuel equals to 0.0040124501 kmol/s of fuel.

and as 1 kmol of air weighs 28.97 kg/kmol, then a kmols of air per 1 kmol of fuels equals [0.0040124501*28.97]*a = 0.1162406782*a kg/s of air for 0.07 kg/s fuel

$$\dot{m}_1 = (1 + 3.76) \cdot a_1 \cdot 0.1162406782 \ [\text{kg/s}] \tag{57}$$

$$\dot{m}_1 + \dot{m}_2 = (1 + 3.76) \cdot a_2 \cdot 0.1162406782 \ [\text{kg/s}] \tag{58}$$

$$\dot{m}_1 + \dot{m}_2 + \dot{m}_3 = (1 + 3.76) \cdot a_3 \cdot 0.1162406782 \ [\text{kg/s}] \tag{59}$$

Appendix A

From Table 1.7a we can give estimated initial values of K to our program:
$K_1 = K_{P,5}$ 2 / $K_2 = K_{P,1}$ 2 / $K_3 = K_{P,2}$ 2 / $K_4 = K_{P,3}$ 2 / $K_5 = (K_{P,10} / K_{P,9})$ 2 / $K_6 = (K_{P,3}$ / sqrt($K_{P,4}$)) 4

$$K_{1,1} = 3.076 \times 10^{-23} \tag{60}$$

$$K_{1,2} = 4.467 \times 10^{-25} \tag{61}$$

$$K_{1,3} = 2.779 \times 10^{-32} \tag{62}$$

$$K_{2,1} = 2.000 \times 10^{-9} \tag{63}$$

$$K_{2,2} = 2.099 \times 10^{-10} \tag{64}$$

$$K_{2,3} = 3.133 \times 10^{-14} \tag{65}$$

$$K_{3,1} = 2.177 \times 10^{-8} \tag{66}$$

$$K_{3,2} = 2.965 \times 10^{-9} \tag{67}$$

$$K_{3,3} = 1.225 \times 10^{-12} \tag{68}$$

$$K_{4,1} = 0.1514 \tag{69}$$

$$K_{4,2} = 0.1086 \tag{70}$$

$$K_{4,3} = 0.02965 \tag{71}$$

$$K_{5,1} = 2.138 \times 10^{8} \tag{72}$$

$$K_{5,2} = 2.547 \times 10^{9} \tag{73}$$

$$K_{5,3} = 4.325 \times 10^{13} \tag{74}$$

$$K_{6,1} = 9.204 \times 10^{-12} \tag{75}$$

$$K_{6,2} = 5.176 \times 10^{-13} \tag{76}$$

$$K_{6,3} = 6.576 \times 10^{-18} \tag{77}$$