PART 2

Equations

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

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

end $getenthalpy$ (3)

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

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

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

end h_g (7)

$$T_{air} = 460\ [\mathrm{K}] \tag{8}$$

$$T_{fuel} = 430\ [\mathrm{K}] \tag{9}$$

$$T_{final,1} = 1700\ [\mathrm{K}] \tag{10}$$

$$T_{final,2} = 1600\ [\mathrm{K}] \tag{11}$$

$$T_{final,3} = 1300\ [\mathrm{K}] \tag{12}$$

$$P = 1000\ [\mathrm{kPa}] \tag{13}$$

$$P_{ref} = 100\ [\mathrm{kPa}] \tag{14}$$

$$R = R\# \tag{15}$$

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

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

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

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

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

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

$$1.1 = b_i + n_i \tag{22}$$

$$4.2 = 2 \cdot c_i + j_i + k_i + 2 \cdot m_i \tag{23}$$

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

$$3.76 \cdot 2 \cdot a_i = 2 \cdot d_i + g_i \tag{25}$$

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

end (56)

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

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

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

$$K_{1,1} = 3.076 \times 10^{-23} \quad (60)$$

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

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

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

$$K_{2,2} = 2.099 \times 10^{-10} \quad (64)$$

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

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

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

$$K_{3,3} = 1.225 \times 10^{-12} \quad (68)$$

$$K_{4,1} = 0.1514 \quad (69)$$

$$K_{4,2} = 0.1086 \quad (70)$$

$$K_{4,3} = 0.02965 \quad (71)$$

$$K_{5,1} = 2.138 \times 10^{8} \quad (72)$$

$$K_{5,2} = 2.547 \times 10^{9} \quad (73)$$

$$K_{5,3} = 4.325 \times 10^{13} \quad (74)$$

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

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

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

PART II

total mass flowrate at each stage - accounting for the initial mass of the fuel

$$\dot{m}_{cumulative,1} = 0.07 \ [\mathrm{kg/s}] + \dot{m}_1 \quad (78)$$

$$\dot{m}_{cumulative,2} = 0.07 \ [\mathrm{kg/s}] + \dot{m}_1 + \dot{m}_2 \quad (79)$$

$$\dot{m}_{cumulative,3} = 0.07 \ [\mathrm{kg/s}] + \dot{m}_1 + \dot{m}_2 + \dot{m}_3 \quad (80)$$

geometric specifications of each PFR

$$L_1 = 0.12 \ [\mathrm{m}] \quad (81)$$

$$L_2 = 0.34 \ [\mathrm{m}] \quad (82)$$

$$L_3 = 0.3 \ [\mathrm{m}] \quad (83)$$

$$A_L = 0.0471 \ \left[\mathrm{m}^2\right] \quad (84)$$

duplicate $z = 1,\ 3$ (85)

I used the compressibility factor (assumed all of our products were N2) to improve the accuracy of our equation of state. Dont worry, the max value Z ever takes in this problem is 1.003

$$Z_{factor,z} = \mathrm{Z}\left(Nitrogen,\ \mathrm{T} = T_{final,z},\ \mathrm{P} = P\right) \tag{86}$$

Calculating the residence time from the mass flowrates and the lengths of each PFR

The 0.0040124501 is included because n_{tot} is our total mole count per 1 mole of fuel. but we have 0.0040124501 moles of fuel per second in reality, so our number must be corrected

$$\rho_z \cdot ((n_{tot,z} \cdot 0.0040124501) \cdot Z_{factor,z} \cdot R \cdot T_{final,z}) = (P \cdot \dot{m}_{cumulative,z}) \tag{87}$$

$$v_z \cdot (\rho_z \cdot A_L) = \dot{m}_{cumulative,z} \tag{88}$$

$$t_{r,z} \cdot v_z = L_z \tag{89}$$

Finding the concentrations of relevant species at each stage using their corresponding mole fractions found in part 1 and the equation of state Pv=ZRT

$$C_{N2,z} = y_{N2,z} \cdot \frac{P}{(Z_{factor,z} \cdot R \cdot T_{final,z})} \tag{90}$$

$$C_{O2,z} = y_{O2,z} \cdot \frac{P}{(Z_{factor,z} \cdot R \cdot T_{final,z})} \tag{91}$$

$$C_{O,z} = y_{O,z} \cdot \frac{P}{(Z_{factor,z} \cdot R \cdot T_{final,z})} \tag{92}$$

$$C_{N,z} = y_{N,z} \cdot \frac{P}{(Z_{factor,z} \cdot R \cdot T_{final,z})} \tag{93}$$

$$C_{H,z} = y_{H,z} \cdot \frac{P}{(Z_{factor,z} \cdot R \cdot T_{final,z})} \tag{94}$$

$$C_{OH,z} = y_{OH,z} \cdot \frac{P}{(Z_{factor,z} \cdot R \cdot T_{final,z})} \tag{95}$$

Zeldovich mechanism rate coefficients given to us as an input

$$k_{N1,f,z} = 1.8\ \left[\mathrm{m^3/kmol{\cdot}s}\right] \cdot (1011) \cdot \exp\left(-38370\ [\mathrm{K}] \frac{}{T_{final,z}}\right) \tag{96}$$

$$k_{N1,r,z} = 3.8\ \left[\mathrm{m^3/kmol{\cdot}s}\right] \cdot (1010) \cdot \exp\left(-425\ \frac{[\mathrm{K}]}{T_{final,z}}\right) \tag{97}$$

$$k_{N2,f,z} = 1.8\ \left[\mathrm{m^3/kmol{\cdot}s{\cdot}K}\right] \cdot T_{final,z} \cdot (107) \cdot \exp\left(-4680\ \frac{[\mathrm{K}]}{T_{final,z}}\right) \tag{98}$$

$$k_{N2,r,z} = 3.8\ \left[\mathrm{m^3/kmol{\cdot}s{\cdot}K}\right] \cdot T_{final,z} \cdot (106) \cdot \exp\left(-20820\ \frac{[\mathrm{K}]}{T_{final,z}}\right) \tag{99}$$

$$k_{N3,f,z} = 7.1\ \left[\mathrm{m^3/kmol{\cdot}s}\right] \cdot (1010) \cdot \exp\left(-450\ \frac{[\mathrm{K}]}{T_{final,z}}\right) \tag{100}$$

$$k_{N3,r,z} = 1.7\ \left[\mathrm{m^3/kmol{\cdot}s}\right] \cdot (1011) \cdot \exp\left(-24560\ \frac{[\mathrm{K}]}{T_{final,z}}\right) \tag{101}$$

Rate of Reactions for the Zeldovich mechanism

$$RR_{1,z} = (k_{N1,f,z} \cdot C_{O,z} \cdot C_{N2,z}) - (k_{N1,r,z} \cdot C_{NO,z} \cdot C_{N,z}) \tag{102}$$

$$RR_{2,z} = (k_{N2,f,z} \cdot C_{N,z} \cdot C_{O2,z}) - (k_{N2,r,z} \cdot C_{NO,z} \cdot C_{O,z}) \tag{103}$$

$$RR_{3,z} = (k_{N3,f,z} \cdot C_{N,z} \cdot C_{OH,z}) - (k_{N3,r,z} \cdot C_{NO,z} \cdot C_{H,z}) \tag{104}$$

Rate of change of the concenration for NO

$$dC_{NOdt,z} = RR_{1,z} + RR_{2,z} + RR_{3,z} \tag{105}$$

$$\text{end} \tag{106}$$

Integrating the rate of change of the NO concenration to get the NO concentration at each stage of the combustion

$$C_{NO,1} = 0 \tag{107}$$

$$C_{NO,2} = C_{NO,1} + \int_0^{t_{r,1}} dC_{NOdt,1} \, \mathrm{d}Time_1 \tag{108}$$

$$C_{NO,3} = C_{NO,2} + \int_0^{t_{r,2}} dC_{NOdt,2} \, \mathrm{d}Time_2 \tag{109}$$

$$C_{NO,4} = C_{NO,3} + \int_0^{t_{r,3}} dC_{NOdt,3} \, \mathrm{d}Time_3 \tag{110}$$

Total NO emission of the combustor in ppm

$$PPM \cdot P = C_{NO,4} \cdot Z_{factor,3} \cdot R \cdot T_{final,3} \cdot \left(10^6\right) \tag{111}$$

Final note: in my research, I have found that a 0.13 PPM value for NO in a gas turbine is very unlikely but plausible. So I stopped looking for problems in my own code and put the blame on unrealistic data
but it could be due to a difference in defining PPM based on molar fractions or volumetric fractions (or even mass fractions)