ME301A (First Sem, 2017 – 18)

Assignment 1

Due date: Aug 31 (Thursday)

Submit problem no. 2, 3, 4, 7 only (remaining are for practice)

1) A mixture of 40% by volume methane, CH_4, and 60% by volume propane, C_3H_8, is burned completely with stoichiometric air. Determine the Air/Fuel ratio on a mass and on a mole basis. Determine the lower and upper heating value of the mixture during the stoichiometric combustion

2) Consider the (a) constant pressure (b) constant volume, adiabatic combustion of a Methyl alcohol (CH_3OH) with air, at temperature 25^0C. Determine the adiabatic flame temperature and plot it for at least 10 values of equivalence ratio ranging from lean to rich mixture. You may write a MATLAB code. Use polynomial expressions for species specific heat.

3) Liquid octane (C_8H_{18}) enters the combustion chamber of a gas turbine at 25^0C and air enters from the compressor at 250^0C. It is determined that 98% of the carbon in the fuel burns to form CO_2 and remaining 2% buns to form CO. What amount of excess air will be required if the temperature of the products is to be limited to 850^0C?

4) Calculate the equilibrium composition for the reaction $H_2 + 1/2O_2 = H_2O$, when the ratio of the number of moles of elemental hydrogen to elemental oxygen is unity. The temperature is 2000K and pressure is 2 atm. Determine the equilibrium composition if O_2 further dissociates in to O atoms, $O_2 = 2O$.

5) Consider the water-shift reaction $CO_2 + H_2 = CO + H_2O$. Assume that the equilibrium constant k(T) is k(1100K) = 1 and k (2100K) = 10. Further assume that the global forward reaction rate coefficient is $K_f = AT^n e^{\frac{-T_A}{T}}$ where $T_A = 15000$ K, n=1/2 and A=$10^{10} cm^3 mol^{-1} s^{-1}$. Estimate the global reverse rate coefficient k_r at 1600 K. (The water gas shift reaction is a global description of the reaction sequence $CO_2 + H \rightarrow CO + OH, H_2 + OH \rightarrow H_2O + H$.)

6) Consider the following elementary reactions of the Hydrogen-Chlorine combustion system:

$$Cl_2 + M \xrightarrow{k_1} Cl + Cl + M$$

$$Cl + H_2 \xrightarrow{k_2} HCl + H$$

$$H + Cl_2 \xrightarrow{k_3} HCl + Cl$$

$$Cl + Cl + M \xrightarrow{k_4} Cl_2 + M$$

Derive the following rate expression by assuming quasi-steady state

$$\frac{d[\mathrm{HCL}]}{dt} = 2k_2\sqrt{\frac{k_1}{k_4}}[\mathrm{Cl_2}]^{0.5}[\mathrm{H_2}]$$

7) Assume a simple reaction chain consisting of two elementary steps:

$$S_1 \xrightarrow{k_{12}} S_2 \xrightarrow{k_{23}} S_3$$

(a) Derive the rate laws for each species, S1, S2 and S3.

(b) If S_2 is very reactive and has a short chemical time scale ($k_{23} >> k_{12}$), S_2 is consumed as soon as it is produced. Thus, consumption and production rates of S2 can be assumed to approximately balance $\frac{\mathrm{d}[\mathrm{S}_2]}{\mathrm{dt}} \approx 0$ and such an assumption is called the quasi-steady state assumption. Simplify the expression obtained in (1) by applying the quasi-steady state assumption.

(c) Plot species concentrations (you may normalize concentration by $[S_1]_{t=0}$) vs. time.