Tutorial 1

1. Consider a mixture of N_2 and Ar in which there are three as many moles of N_2 as there are moles of Ar. Determine the mole fraction of N_2 and Ar, the molecular weight of the mixture, the mass fraction of N_2 and Ar, and the molar concentration of N_2 in kmol/m^3 for a temperature of 500 K and a pressure of 250 kPa.

   Ans: a) 0.75, 0.25; b) 31kg/kmol; c) 0.677, 0.323; d) 0.045kmol/m^3

2. Determine the absolute enthalpy in J/kmol$_{mix.}$ Of a mixture of CO_2 and O_2 where χ_{CO2} = 0.10 and χ_{O2} = 0.90 at a temperature of 400K.

   Ans: -36,226kJ/kmol$_{mix}$

3. Consider a stoichiometric mixture of isooctane and air. Calculate the enthalpy of the mixture at the standard state temperature (298.15) on a per kmol of fuel basis (kJ/kmol$_{fuel}$), on a per kmol of mixture basis (kJ/kmol$_{mix}$) and on a per mass of mixture basis (kJ/kg$_{mix}$).

   Ans: -224,109kJ/kmol$_{C8H18}$, -3697.8kJ/kmol$_{mix}$; -122.24kJ/kg$_{mix}$

4. The lower heating value of vapor n-decane is 44,597 kJ/kg at T = 298K. The enthalpy of vaporization of n-decane is 276.8 kJ/kg of decane. The enthalpy of vaporization of water at 298K is 2442.2kJ/kg of water.
   a. Determine the lower heating value of liquid n-decane. Use the units of kJ/kg n-decane to express your results.
   b. Determine the higher heating value of vapor n-decane at 298K.

   Ans: a) 44,320kJ/kg; b) 48002.3kJ/kg

5. The higher heating value for liquid octane (C_8H_{18}) at 298K is 47,893 kJ/kg and the heat of vaporization is 363 kJ/kg. Determine the enthalpy of formation at 298K for octane vapor.

   Ans: -219906 kJ/kmol

6. Determine the adiabatic flame temperature for constant pressure combustion of a stoichiometric propane-air mixture assuming reactants at 298K, no dissociation of the products, and constant specific heats evaluated at 298K.

   Ans: 2879.3K

7. A furnace, operating at 1atm, uses preheated air to improve its fuel efficiency. Determine the adiabatic flame temperature when the furnace is run at a mass air fuel ratio of 18 for air preheated to 800K. the fuel enters at 450K. Assume the following simplified thermodynamic properties:
   T_{ref} = 300K, $MW_{fuel} = MW_{air} = MW_{prod}$ = 29kJ/mol, $C_{p,fuel}$ = 3500 J/kg-K; $C_{p,air} = C_{p,prod.}$ = 1200 J/kg-K, $h^0_{f,air} = h^0_{f,prod} = 0$, $h^0_{f,fuel} = 1.16\times10^9 J/kmol$

   Ans: 2551K

8. Consider the equilibrium reaction $O_2 \leftrightarrow 2O$ in a closed vessel. Assume the vessel contains 1mol of O_2 when there is no dissociation. Calculate the mole fraction of O_2 and O for the following conditions:
    a. T = 2500K, P = 1atm
    b. T = 2500K, P = 3atm

Ans: a) x_O=0.0143, x_{O2}=0.9857; b) x_O=0.00825, x_{O2}=0.99175

9. Consider the equilibrium reaction $CO_2 \leftrightarrow CO + \frac{1}{2}O_2$. At 10atm and 3000K, the equilibrium mole fractions of a particular mixture of CO_2, CO, and O_2 are 0.6783, 0.2144 and 0.1073, respectively. Determine the equilibrium constant K_p for this reaction.

Ans: 0.327

10. Calculate the equilibrium composition for the reaction $H_2 + \frac{1}{2}O_2 \leftrightarrow H_2O$ when the ratio of the number of moles of elementary hydrogen to elementary oxygen is unity. The temperature is 2000K, and the pressure is 1atm.

Ans: x_{H20}=0.6662; x_{O2}=0.3334; x_{H2}=0.00033

11. Consider the constant-pressure adiabatic combustion of a stoichiometric air fuel mixture where $(A/F)_{stoic}$ = 15. Assume the following simplified properties for the fuel, air and products with T_{ref} = 300K:

	Fuel	Air	Products
C_p (J/kg-K)	3500	1200	1500
$h^0_{f,300}$ (J/kg)	2×10^7	0	-1.25×10^6

    a. Determine the adiabatic flame temperature for a mixture initially at 600K.
    b. Determine the heating value of the fuel at 600K. Give units.

Ans: a) 2235K; b) 39.25 MJ/kg_{fuel}

12. Propane burns in a premixed flame at an air-fuel ratio (mass) of 18:1. Determine the equivalence ratio.

Ans: 0.87

13. Methyl alcohol (CH_3OH) burns with excess air at an air-fuel ratio (mass) of 8.0. Determine the equivalence ratio and the mole fraction of CO_2 in the product mixture assuming complete combustion, i.e., no dissociation.

Ans: 0.674, 0.099

14. Consider a fuel which is an equimolar mixture of propane (C_3H_8) and natural gas (CH_4). Write out the complete stoichiometric combustion reaction for this fuel burning with air and determine the stoichiometric fuel-air ratio on a molar basis. Also, determine the molar air-fuel ratio for combustion at an equivalence ratio of 0.8.

Ans: 0.06, 0.048

15. Consider a gas phase reaction $N_2O_4 \leftrightarrow 2NO_2$ occurring in an isothermal and isobaric reactor maintained at 298K and 1 bar. The standard Gibbs energy change of the reaction

at 298K is $\Delta G^{\circ}_{298} = 5253 \frac{J}{mol}$. The standard states are those of pure ideal gases at 1bar. The equilibrium mixture in the reactor behaves as an ideal gas. The value of the universal gas constant is $8.314 \frac{J}{mol\ K}$. If one mole of pure N_2O_4 is initially charged to the reactor, then find the fraction of N_2O_4 that decomposes into NO_2 at equilibrium.

Ans: 0.17

16. Carbon monoxide (CO) reacts with hydrogen sulphide (H_2S) at a constant temperature of 800K and a constant pressure of 2bar as: $CO + H_2S \leftrightarrow COS + H_2$. The gibbs free energy of the reaction $\Delta G^{\circ}_{rxn} = 22972.3 \frac{J}{mol}$ and universal gas constant is $8.314 \frac{J}{mol\ K}$. Both the reactants and products can be assumed to be ideal gases. If initially only 4mol of H_2S and 1mol of CO are present, find the extent of reaction (in mol) at equilibrium.

Ans: 0.288

17. The reversible reaction of t-butyl alcohol (TBA) and ethanol (EtOH) to ethyl-t-butyl ether (ETBE) is $TBA + EtOH \leftrightarrow ETBE + Water$. The equilibrium constant for this reaction is K_c=1. Initially, 74g of TBA is mixed with 100g of aqueous solution containing 46 weight% ethanol. The molecular weights are: 74g/mol for TBA, 46 g/mol for EtOH, 102g/mol for ETBE and 18g/mol for water. Find the mass of ETBE at equilibrium.

Ans: 20.4g

18. A feedstock of pure n-butane is cracked at 750K and 1.2 bar to produce olefins. Only two reactions have favourable equilibrium conversions at these conditions:

$$C_4H_{10} \rightarrow C_2H_4 + C_2H_6 \quad (I)$$
$$C_4H_{10} \rightarrow C_3H_6 + CH_4 \quad (II)$$

If these reactions reach equilibrium, what is the product composition? The equilibrium constants at 750K are found to be $K_I = 3.856$ and $K_{II} = 268.4$

Ans: $x_{C4H10} = 0.001$, $x_{C2H4} = x_{C2H6} = 0.0534$ and $x_{C3H6} = X_{CH4} = 0.4461$