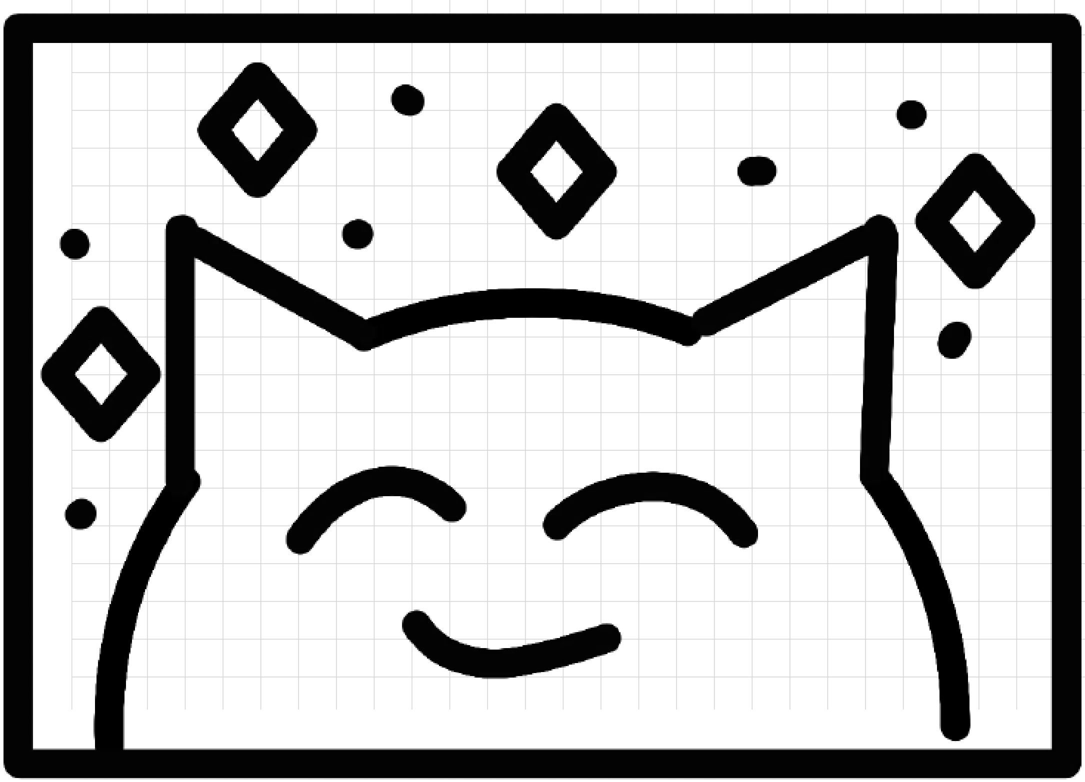
MAE 112

HW 2

TRIET



1. Calculate theoretical (ideal) flame temperature for methane (CH_4) in stoichiometric ratio with enriched air (50% O_2, 50% N_2 by volume). Pressure is constant at 15 atm and the initial temperature is 298 K.

Stoichiometric reaction:

$$a\,CH_4 + b(O_2 + N_2) \longrightarrow c\,CO_2 + d\,H_2O + e\,N_2$$

$$1\,CH_4 + 2(O_2 + N_2) \longrightarrow 1\,CO_2 + 2\,H_2O + 2\,N_2$$

Mole number (n), heat of formation ($h_{f,m}$) and specific heats ($c_{p,m}$)

	n	$h_{f,m}$ [J/mol]	$C_{p,m}$ [J/mol-K]
CH_4	1	-74 831	N/A
O_2	2	0	N/A
N_2	2	0	34.805
CO_2	1	-393 546	58.292
H_2O	2	-241 845	47.103
N_2	2	0	34.805

Energy balance:

$$\sum_{\text{reactants}} n\left(h_{f,m} + \int_{T_{ref}}^{T_i} C_{p,m}\,dT\right) = \sum_{\text{Products}} n\left(h_{f,m} + \int_{T_{ref}}^{T_{final}} C_{p,m}\,dT\right)$$

$$n_{CH_4}(h_{f,CH_4} + 0) + 0 + 0 = n_{CO_2}(h_{f,CO_2} + C_{p,CO_2}\Delta T) + n_{H_2O}(h_{f,H_2O} + C_{p,H_2O}\Delta T) + n_{N_2}(0 + C_{p,N_2}\Delta T)$$

$$n_{CH_4} \cdot h_{f,CH_4} = n_{CO_2}\,h_{f,CO_2} + n_{H_2O}\,h_{f,H_2O} + \Delta T\left(n_{O_2}C_{p,O_2} + n_{H_2O}C_{p,H_2O} + n_{N_2}C_{p,N_2}\right)$$

$$\Delta T = \frac{n_{CH_4} \cdot h_{f,CH_4} - (n_{CO_2}\,h_{f,CO_2} + n_{H_2O}\,h_{f,H_2O})}{n_{O_2}C_{p,O_2} + n_{H_2O}C_{p,H_2O} + n_{N_2}C_{p,N_2}}$$

$$T_f - 298 = \frac{1 \times (-74\,831) - [1 \times (-393\,546) + 2(-241\,845)]}{1 \times 58.292 + 2 \times 47.103 + 2 \times 34.805}$$

$$\boxed{T_f = 3910.68\ [K]}$$

3. (a) Calculate AF at stoichiometric condition (AF_{st}) for ethyl alcohol C_2H_5OH (aka ethanol) initially at 550 ° R burning in air at 20 atmospheres of pressure. AF is the ratio of mass flow of air to mass flow of fuel. Also, calculate FA = 1/ AF for the same condition.

(b) Calculate AF and $\Phi = AF_{st} / AF = FA/ FA_{st}$ for ethyl alcohol and 50% excess air at the same conditions.

Molecular weight of single element:

$$W_C = 12.011 \left[\frac{g}{mol}\right] \quad W_H = 1 \left[\frac{g}{mol}\right] \quad W_O = 16 \left[\frac{g}{mol}\right] \quad W_N = 14\left[\frac{g}{mol}\right]$$

$$a\, C_2H_5OH + b(O_2 + 3.76\, N_2) \rightarrow c\, CO_2 + d\, H_2O + e\, N_2$$

$$1\, C_2H_5OH + 3(O_2 + 3.76\, N_2) \rightarrow 2\, CO_2 + 3\, H_2O + 11.28\, N_2$$

ⓐ Air to fuel ratio:

$$A/F = \frac{m_{Air}}{m_{Fuel}} = \frac{3 \times (2\times16 + 3.76 \times 2\times14)}{1\times(2\times12.011 + 5 + 16 + 1)} = \boxed{8.9488}$$

Fuel to air ratio:

$$F/A = 1 \div A/F = 1 \div 8.9488 = \boxed{0.1117}$$

ⓑ

Air mole : $1.5\, n_{air} = 1.5 \times 3 = 4.5$

$$1\, C_2H_5OH + 4.5(O_2 + 3.76\, N_2) \rightarrow \cdots$$

Air to fuel ratio:

$$A/F = \frac{m_{Air}}{m_{Fuel}} = \frac{4.5\times(2\times16 + 3.76 \times 2\times14)}{1\times(2\times12.011 + 5 + 16 + 1)} = \boxed{13.4231}$$

Fuel to air ratio:

$$F/A = 1 \div A/F = 1 \div 13.4231 = \boxed{0.0745}$$

Equivalent ratio:

$$\Phi = \frac{A/F_{\text{stoichimometry}}}{A/F_{\text{at 50\% excess air}}} = \frac{8.9488}{13.4231} = \boxed{0.6667}$$

4. (a) Establish the equations which can be employed for the calculation of the equilibrium composition and the flame temperature when one mole of propane C_3H_8 burns adiabatically at a constant pressure of ten atmospheres. The mixture is lean with 75% excess air. Both air and fuel enter at a temperature of 800°R. Consider the products to be CO_2, CO, H_2O, H_2, O_2, and N_2 only. Write all the required equations with known quantities and parameters substituted into the equation. Identify the unknowns. Propane is gaseous at room temperature. Explain what would be different in the analysis if propane entered at a lower temperature in liquid form.
(b) Use the computer software to calculate the final flame temperature and concentrations of the products with the gaseous propane fuel.
(c) For the adiabatic situation with gaseous fuel described in Part a, establish the equations to solve for the theoretical (ideal) temperature and composition. What are the products in this case? Again, write the necessary equations, identify the known quantities, and identify the unknowns. Solve the equations for the final temperature and composition. Which of the two temperatures from 2b and 2c is larger? Why?

(a) Stoichiometric reaction:

$$1\ C_3H_8 + 5(O_2 + 3.76 N_2) \rightarrow 3CO_2 + 4H_2O + 18.8 N_2$$

75 % excess air:

$$C_3H_8 + 8.75(O_2 + 3.76 N_2) \rightarrow a\,CO_2 + b\,H_2O + 32.9\,N_2 + c\,CO + d\,H_2 + e\,O_2$$

C: $3 = a + c$

H: $8 = 2b + 2d$

O: $17.5 = 2a + b + c + 2e$

N: Aldready balanced

Two dissociation:

$$CO_2 \longleftrightarrow CO + \frac{1}{2} O_2$$

$$K_1 = \frac{X_{CO} X_{O_2}^{1/2}}{X_{CO_2}} = P^{-1/2} K_{P1}(T_f)$$

$$H_2O \longleftrightarrow H_2 + \frac{1}{2} O_2$$

$$K_2 = \frac{X_{H_2} X_{O_2}^{1/2}}{X_{H_2O}} = P^{-1/2} K_{P2}(T_f)$$

Energy conservation:

$$\sum_{reactants} n_m \left(h_{f,m} + \int_{T_{ref}}^{T_i} c_{p,m}\, dT \right) = \sum_{products} n_m \left(h_{f,m} + \int_{T_{ref}}^{T_f} c_{p,m}\, dT \right)$$

(c) Stoichiometric reaction:

$$1\ C_3H_8 + 5\,(O_2 + 3.76\ N_2) \longrightarrow 3\,CO_2 + 4\ H_2O + 18.8\ N_2$$

75 % excess air:

$$1\,C_3H_8 + 8.75(O_2 + 3.76\,N_2) \longrightarrow 3\,CO_2 + 4\ H_2O + 32.9\ N_2 + 3.75\ O_2$$

From textbook / internet:

	$h_{f,m}$ [J/mol]	$c_{p,m}$ [J/mol-K]
C_3H_8	−103847	73.920
O_2	0	34.88
N_2	0	32.676
H_2O	−241845	41.103
CO_2	−393546	54.299
CO	−110500	28.56
H_2	0	14.5
O_2	0	34.88
N_2	0	32.676

Energy conservation:

$$\sum_{reactants} n_m \left(h_{f,m} + \int_{T_{ref}}^{T_i} c_{p,m}\, dT \right) = \sum_{products} n_m \left(h_{f,m} + \int_{T_{ref}}^{T_f} c_{p,m}\, dT \right)$$

$T_i = 800\,[°R] = 444\,[K]$ $\quad T_{ref} = 298.15\,[K]$

$\Rightarrow T_f = 1769.7475\,[K]$

Less than part (b) $T_f = 1765.7\,[K]$

$\Rightarrow$ Excess conditions decrease T_f