

JQ.2.33.Soln

October 6, 2014

(2.33) A gaseous mixture of 2% (by volume) acetone and 4% ethanol in air is at 25°C and a pressure of 1 atm.

Data

Acetone ($\text{C}_3\text{H}_6\text{O}$) has $\Delta h_c = 1786 \text{ kJ}/(\text{gmol})$

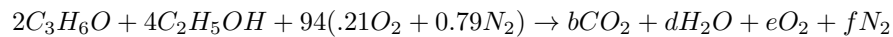
Ethanol ($\text{C}_2\text{H}_5\text{OH}$) has $\Delta h_c = 1232 \text{ kJ}/(\text{gmol})$

Atomic weights are given. Assume that the mass specific heat at constant pressure for each species is $c_{p,i} = 1 \text{ kJ}/(\text{kgK})$.

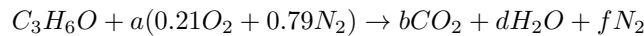
- (a) For a constant pressure reaction, calculate the partial pressure of the oxygen in the product mixture.
- (b) Determine the adiabatic flame temperature of this mixture.
- (c) If this mixture were initially at 400°C , what will the resultant adiabatic flame temperature be?

Setup.

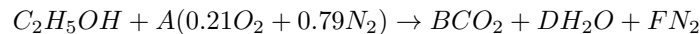
- (a) The hard way to solve this problem is to try to balance the elements for the combined mixture. By this I mean:



It is easier to do each fuel separately in a stoichiometric mixture:



and



Once you know the stoichiometric reactions, add them together multiplying by the respective mole fraction (use Amagat's law). Check if there is excess air, excess fuel, or balanced.

For $\text{C}_3\text{H}_6\text{O}$ we perform the balances:

$$\text{C} : 3 = b; \text{H} : 6 = 2d; \text{O} : 1 + 2 \times 0.21 \times a = 2b + d; \text{N} : 0.79 \times a = f$$

$$b=3; d=3; f=0.79a$$

In [41]: `b=3; d=3; a=(2*b+d-1.)/(2.*0.21); f=0.79*a; a`

Out[41]: 19.047619047619047

In [42]: `a*.21`

Out[42]: 4.0

The balanced equation for acetone is $\text{C}_3\text{H}_6\text{O} + 19.05(0.21\text{O}_2 + 0.79\text{N}_2) \rightarrow 3\text{CO}_2 + 3\text{H}_2\text{O} + 15.05\text{N}_2$

For $\text{C}_2\text{H}_5\text{OH}$ we perform the balances:

$$\text{C} : 2 = B; \text{H} : 6 = 2D; \text{O} : 1 + 2 \times 0.21 \times A = 2B + D; \text{N} : 0.79 \times A = F$$

$$B=2; D=3; F=1.58$$

In [35]: B=2; D=3; A=(2*B+D-1.)/(2.*0.21); F=0.79*A; F

Out[35]: 11.285714285714286

The balanced equation for ethanol is $C_2H_5OH + 14.29(0.21O_2 + 0.79N_2) \rightarrow 2CO_2 + 3H_2O + 11.29N_2$
When we consider a 2% acetone and 4% ethanol mixture the amount of stoichiometric air is found from:

$$2 \times (C_3H_6O + 19.05(0.21O_2 + 0.79N_2)) + 4 \times (C_2H_5OH + 14.29(0.21O_2 + 0.79N_2))$$

the number of moles of air is $2 \times 19.05 + 4 \times 14.29$

In [36]: 2.*19.05+4.*14.29

Out[36]: 95.25999999999999

The number of moles of stoichiometric air is 95.3 while the available number of moles of air is 94. We see that the reaction is oxygen deficient or fuel rich. There is no oxygen on the product side of the reaction and $P_{O_2} = 0$.

- (b) We are generalizing the adiabatic flame temperature model to include multiple fuels. Recall that the flame temperature using a mass basis formulation is found from.

$$0 = \sum_i m_{F,i} \Delta h_{c,i} + \sum_i m_i c_{p,i} (T_R - 25) - \sum_j m_j c_{p,j} (T_P - 25)$$

This mass form is particularly useful for a case in which the reactants are already at $25^\circ C$ since the sum on the reactant enthalpies is then zero. Next we can define a mass averaged specific heat capacity as:

$$m_T \bar{c} = \sum m_i c_i$$

$$0 = m_{F,1} \Delta h_{c,1} + m_{F,2} \Delta h_{c,2} - m_T \bar{c} (T_P - 25)$$

$$T_P = 25 + \frac{m_{F,1}}{m_T} \frac{\Delta h_{c,1}}{\bar{c}} + \frac{m_{F,2}}{m_T} \frac{\Delta h_{c,2}}{\bar{c}} = 25 + Y_{F,1} \frac{\Delta h_{c,1}}{\bar{c}} + Y_{F,2} \frac{\Delta h_{c,2}}{\bar{c}}$$

In [37]: Dhc_mole_AC=1786; MW_AC= 3*12+6+16; Dhc_mole_ET=1232; MW_ET= 2*12+6+16; Dhc_mass_AC= Dhc_mole_

In [38]: c_mix=32.7/28. ; Y_AC= 2.*MW_AC/(2.*MW_AC+4.*MW_ET+94.*28.8); Y_ET= 4.*MW_ET/(2.*MW_AC+4.*MW_ET

In [39]: T_P=25. + Y_AC*Dhc_mass_AC*1000./c_mix + Y_ET*Dhc_mass_ET*1000./c_mix ; T_P

Out[39]: 2378.088571119425

The calculation above predicts a product temperature of $2378^\circ C$.

- (c) Use the same approach as in part (b). We see thwe will simply increase the initial temperature to $400^\circ C$. In practice, the specific heat capacity should be adjusted to account for the higher product temperature.

In [40]: T_P400=400. + Y_AC*Dhc_mass_AC*1000./c_mix + Y_ET*Dhc_mass_ET*1000./c_mix ; T_P400

Out[40]: 2753.088571119425

Using a crude approximation that the specific heat capacity does not increase, we find that the product temperature is $2753^\circ C$.