# JQ.2.13.soln

September 19, 2014

2.13 (a)Write the balanced chemical equation for stocihiometric combustion of benzene ($C_6H_6$). Assume complete combustion. Calculate the mass of air required to burn a unit mass of combustible.

You know at this point how to use an element balance to solve this problem.

$$C_6H_6 + a(O_2 + 3.76N_2) \rightarrow bCO_2 + dH_2O + 3.76aN_2$$

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In [151]: nC_R=6.; nH_R=6.; b=nC_R; d=nC_R/2.; a_ST=b+d/2.;

In [152]: b

Out[152]: 6.0

In [153]: a_ST

Out[153]: 7.5

In [154]: d

Out[154]: 3.0
```

The stoichiometric reaction is:

$$C_6H_6 + 7.5(O_2 + 3.76N_2) \rightarrow 6CO_2 + 3H_2O + 28.2N_2$$

b) For a benzene air equivalence ratio of 0.75, write the balanced chemical equaton and calculate the adiabatic flame temperature in air. The initial temperature is 298K and pressure is 1 atm. Assume complete combustion.

Use the definition of the equivalence ratio $\phi = (F/A)/(F/A)_{ST}$ where the $(F/A)$ is the mass of fuel to mass of air at the $\phi = 0.75$ condition. You know the moles of each component species and can easily calculate the molecular weights of the components.

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In [155]: phi= 0.75; MF_ST=6.*12.+6.; MA_ST=a_ST*4.76*28.8;

In [156]: FA_ST=MF_ST/MA_ST; FA=phi*FA_ST; MA=MF_ST/FA; nA= MA/28.8; a=nA/4.76;
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The adiabatic flame temperature is calculated using equation 2.26 with $Q = 0$:

$$-Q = \nu_F \Delta\tilde{h}_c + \sum_i n_i \tilde{c}_{p,i}(T_R - 25) - \sum_j n_j \tilde{c}_{p,j}(T_P - 25)$$

There is an equivalent statement that can be developed using the mass basis.

$$-Q = m_F \Delta h_c + \sum_i m_i c_{p,i}(T_R - 25) - \sum_j m_j c_{p,j}(T_P - 25)$$

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

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

$$0 = m_F \Delta h_c - m_T \bar{c}(T_P - 25)$$

$$T_P = 25 + \frac{m_F}{m_T}\frac{\Delta h_c}{\bar{c}} = 25 + Y_F \frac{\Delta h_c}{\bar{c}}$$

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In [157]: Dhc=40.2; c_mix=32.7/28. ; Y_F=MF_ST/(MF_ST+MA); T_P=25. + Y_F*Dhc*1000/c_mix; T_P
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Out[157]: 1878.0985528081424
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The calculation above predicts a product temperature of $1878^oC$. The mass fraction of benzene was caalculated to be 0.053.

(c) calculate the mole fraction for each product of combustion in part (b). We use the simple definition of mole fraction $X_i = \frac{n_i}{n_T}$. Note that for this fuel lean case $\phi = 0.75$ the reactant mixture has extra air. The products will look like the stoichiometric products diluted with teh excess air.

For $\phi = 0.75$, the global reaction is:

$$C_6H_6 + 7.5(O_2 + 3.76N_2) + 2.5(O_2 + 3.76N_2) \rightarrow 6CO_2 + 3H_2O + 28.2N_2 + 2.5(O_2 + 3.76N_2)$$

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In [158]: n_T=6.+3.+28.2+2.5*4.76; X_CO2=6./n_T; X_H2O=3./n_T; X_O2=2.5/n_T; X_N2=(28.2+2.5*3.76)/n_T;
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In [159]: X_CO2
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Out[159]: 0.12219959266802444
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In [160]: X_H2O
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Out[160]: 0.06109979633401222
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In [161]: X_O2
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Out[161]: 0.05091649694501018
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In [162]: X_N2
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Out[162]: 0.765784114052953
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(d) Benzene often burns incompletely. If 20% of the carbon in the benzene is converted to solid carbon and 5% is being converted to CO during combustion, the remainder being converted to $CO_2$, calcuate the heat released per gram of oxygen consumed. How does this compare with the value in Table 2.3.

We need to revise our model for the consumption of $C_6H_6$.

$$C_6H_6 + a(O_2 + 3.76N_2) \rightarrow bCO_2 + dH_2O + eC + fCO + 3.76aN_2$$

Note that we must include the solid carbon and CO given by the problem statement. We are told that 20% of carbon in benzene is solid and 5% is converted to CO. Of the 6C in benzene, 0.2 is in C and 0.05 is in CO. Use these in the element balance.

$$C_6H_6 + a(O_2 + 3.76N_2) \rightarrow bCO_2 + dH_2O + eC + fCO + 3.76aN_2$$

$e = 6/5$, $f = 6/20$, $6 = b + 6/5 + 6/20$ or $120 = 20b + 24 + 6$, $b = \frac{120-30}{20} = 90/20 = 4.5$ and $2a = 2b + d + f$

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In [163]: e=6./5.; f=6./20.; b=4.5; d=3.; a=b+d/2.+f/2.;
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For

$$C_6H_6 + 6.15(O_2 + 3.76N_2) \rightarrow 4.5CO_2 + 3H_2O + 1.2C + 0.3CO + 23.12N_2$$

We can calculate the heat released per gram of fuel and also per gram of oxygen using heat of formation data. Use equation 2.25 to express the heat of combustion in terms of the heats of formation

$$\Delta\tilde{h}_c = \left(\sum_i \nu_i \Delta\tilde{h}^o_{f,i}\right)_{React} - \left(\sum_j \nu_j \Delta\tilde{h}^o_{f,j}\right)_{Prod}$$

$n_{C6H6} = 1.; n_{CO2} = 4.5.; n_{H2O} = 3.; n_{CO} = 0.3; \Delta h^o_{f,CO2} = -393.5; \Delta h_{f,H2O_{lower}} = -241.8; M_{C6H6} = 78.; \Delta h_{f,CO} = -110.5$

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In [164]: n_C6H6=1.; n_CO2=4.5; n_H2O=3.; n_CO=0.3; hfC6H6= 82.9; hfCO2=-393.5; hfH2O_lower= -241.8; hf(
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In [165]: Dhcmol=hfC6H6 - (n_CO2*hfCO2 + n_H2O*hfH2O_lower + n_CO*hfCO); Dhcmol
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Out[165]: 2612.2000000000003
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The molar heat of combustion for benzene is 1095.1 kJ/mole. We divide by the loecular weight to get the heat of combustion on a mass basis. We divide by the mass of oxygen to get this on a oxygen basis.

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In [166]: DhcmassF=Dhcmol/78.; DhcmassO=Dhcmol/(32.*a); DhcmassO
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Out[166]: 13.273373983739837
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On a mass basis with incomplete combustion, we find that the heat of combustion is $33.5kJ/(g-F)$ and $13.2kJ/(g-Ox)$.