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^oC and a pressure of 1 atm.

Data

Acetone (C_3H_6O) has $\Delta h_c = 1786kJ/(gmol)$

Ethanol (C_2H_5OH) has $\Delta h_c = 1232kJ/(gmol)$

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

(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^oC, 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:

$$2C_3H_6O + 4C_2H_5OH + 94(.21O_2 + 0.79N_2) \rightarrow bCO_2 + dH_2O + eO_2 + fN_2$$

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

$$C_3H_6O + a(0.21O_2 + 0.79N_2) \rightarrow bCO_2 + dH_2O + fN_2$$

and

$$C_2H_5OH + A(0.21O_2 + 0.79N_2) \rightarrow BCO_2 + DH_2O + FN_2$$

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

For C_3H_6O we perform the balances:

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

$b=3; ; d=3; $

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In [41]: b=3; d=3; a=(2*b+d-1.)/(2.*0.21); f=0.79*a; a
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Out[41]: 19.047619047619047
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In [42]: a*.21
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Out[42]: 4.0
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The balanced equation for acetone is $C_3H_6O + 19.05(0.21O_2 + 0.79N_2) \rightarrow 3CO_2 + 3H_2O + 15.05N_2$

For C_2H_5OH we perform the balances:

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

$B=2; ; D=3; $

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In [35]: B=2; D=3; A=(2*B+D-1.)/(2.*0.21); F=0.79*A; F
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Out[35]: 11.285714285714286
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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 $2 \times 19.05 + 4 \times 14.29$

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In [36]: 2.*19.05+4.*14.29
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Out[36]: 95.25999999999999
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The number of moles of stoichiometrhic 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 $P_{O2} = 0$.

(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^oC since the sum on the reactant enthalpies is then zero. Next we can define a mass averaged specific heat capacity as:

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

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

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

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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_
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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_E
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In [39]: T_P=25. + Y_AC*Dhc_mass_AC*1000./c_mix + Y_ET*Dhc_mass_ET*1000./c_mix  ; T_P
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Out[39]: 2378.088571119425
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The calculation above predicts a product temperature of 2378^oC.

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

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In [40]: T_P400=400. + Y_AC*Dhc_mass_AC*1000./c_mix + Y_ET*Dhc_mass_ET*1000./c_mix  ; T_P400
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Out[40]: 2753.088571119425
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Using a crude approximation that the specific heat capacity does not increase, we find that the product temperature is 2753^oC.