Homework II Solution

(1) The efficiency in the ideal case (Carnot cycle) is:

η_{ideal} =1-(300K)/(273K+1300K)=0.81.

Then, the second law efficiency becomes

$$\eta_{II} = \frac{0.5}{0.81} = 0.62$$

LHV of C6H6=40141kJ/kg=3131MJ/kmol (liquid) (Boiling point of C6H6 is 80 C°)

Fuel per available energy is: 1kg/(40140kJ*0.81)=1kmol/2536MJ[1]

Fuel per work produced without sequestration: 1kg/20070kJ=1kmol/1565MJ.

(2)

Compression of air (assumptions: T_1=300K and P_1=1atm)

From $\dfrac{P_2}{P_1} = \left(\dfrac{T_2}{T_1}\right)^{k/(k-1)}$ and $T_2 = T_1 + (T_{2s} - T_1)/\eta_c$

T_2 =832K and P_2=25atm

In the combustion process (assumption: No CO and H2 generation)

$$C_6H_6 + 7.5(O_2 + 3.76N_2) \rightarrow 6CO_2 + 3H_2O + 3.76 \cdot 7.5 \cdot N_2$$
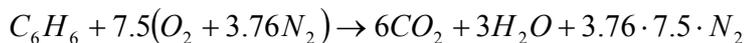
From $H_R(T_2 = 832K) = H_p(T_3)$, we get $T_3 = 2878K$

Note that

$$H_R = \left(\Delta\hat{h}_{f,C_6H_6}^o + \int_{T_o}^{T2} \hat{c}_{p,C_6H_6} dT\right) + 7.5\left(\int_{T_o}^{T2} \hat{c}_{p,O_2} dT + 3.76\int_{T_o}^{T2} \hat{c}_{p,N_2} dT\right)$$

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[1] From Gibbs free energy change, we get a different value of the maximum work:

$w_{max} = -\Delta G = -\Delta h + T\Delta s$ =3131MJ/kmol+300(6 $\hat{s}_{CO2}$ +3 $\hat{s}_{H2O}$ -7.5 $\hat{s}_{O2}$ - $\hat{s}_{C6H6}$)

=3131MJ/kmol+300(6moles*0.214MJ/kmol+3moles*0.189MJ/kmol-7.5moles*0.205MJ/kmol - 0.173MJ/kmol)=3173MJ/kmol.

and

$$H_p = 6\left(\Delta \hat{h}^o_{f,CO_2} + \int_{T_o}^{T_3} \hat{c}_{p,CO_2} dT \right) + 3\left(\Delta \hat{h}^o_{f,H_2O} + \int_{T_o}^{T_3} \hat{c}_{p,H_2O} dT \right) + 3.76 \cdot 7.5 \int_{To}^{T_3} \hat{c}_{p,N_2} dT .$$

While computing the above two expressions, keep in mind that $\hat{c}_p$ is a function of temperature.

In the mixing process

$$6CO_2 + 3H_2O + 3.76 \cdot 7.5 \cdot N_2 + X(O_2 + 3.76N_2) \rightarrow 6CO_2 + 3H_2O + XO_2 + 3.76(7.5 + X)N_2$$
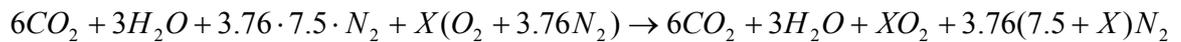
From $H_R(T_3) + H'_R(T_2) = H_P(T_4 = 1573K)$ where

$$H_R(T_3) = 6\left(\Delta \hat{h}^o_{f,CO_2} + \int_{T_o}^{T_3} \hat{c}_{p,CO_2} dT \right) + 3\left(\Delta \hat{h}^o_{f,H_2O} + \int_{T_o}^{T_3} \hat{c}_{p,H_2O} dT \right) + 3.76 \cdot 7.5 \int_{To}^{T_3} \hat{c}_{p,N_2} dT$$

$$H'_R(T_2) = X\left(\int_{T_o}^{T_2} \hat{c}_{p,O_2} dT + 3.76 \int_{To}^{T_2} \hat{c}_{p,N_2} dT \right)$$

and

$$H_P(T_4) = 6\left(\Delta \hat{h}^o_{f,CO_2} + \int_{T_o}^{T_4} \hat{c}_{p,CO_2} dT \right) + 3\left(\Delta \hat{h}^o_{f,H_2O} + \int_{T_o}^{T_4} \hat{c}_{p,H_2O} dT \right) + X \int_{T_o}^{T_4} \hat{c}_{p,O_2} dT +$$
$$3.76 \cdot (7.5 + X) \int_{To}^{T_4} \hat{c}_{p,N_2} dT$$

we get $X = 16.78$.

(3)

Separation work (Assume H₂O is all liquid)

6CO2+24.28*3.76N2+
16.78O2

T=300K,
P=1atm

24.28*3.76N2+
16.78O2

6CO2 (gas)

T=300K,
P=1atm
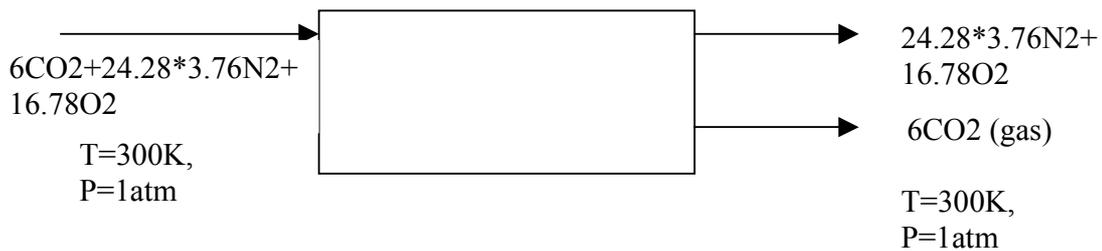
$$-W = n_{CO2}((\hat{h}_{CO2,2} - \hat{h}_{CO2,1}) - T(\hat{s}_{CO2,2} - \hat{s}_{CO2,1})) + n_{N2}((\hat{h}_{N2,2} - \hat{h}_{N2,1}) - T(\hat{s}_{N2,2} - \hat{s}_{N2,1}))$$

$$+ n_{O2}((\hat{h}_{O2,2} - \hat{h}_{O2,1}) - T(\hat{s}_{O2,2} - \hat{s}_{O2,1}))$$

$$= RT(n_{CO2} \log(\frac{1}{X_{CO2,1}}) + (n_{N2} + n_{O2}) \log(\frac{1}{1 - X_{CO2,1}}))$$

$$= 58.6 MJ$$

Required work for separation: 58.6MJ/kmol of C6H6 (3.7% of the work produced in the cycle)

6CO2 (gas)

T1=300K,

P1=1atm

6CO2 (liquid)

T2=300K,

P2=100atm
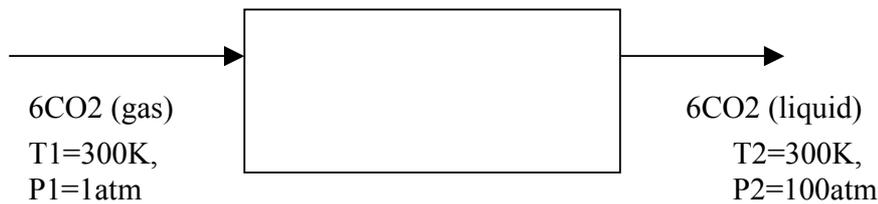
$$-w = ((h_{CO2,2} - h_{CO2,1}) - T(s_{CO2,2} - s_{CO2,1}))$$

$$= (560kJ/kg - 810kJ/kg) - 300K * (3.3kJ/kgK - 4.9kJ/kgK)$$

$$= 230kJ/kg \text{ of } CO_2$$

Since 6kmol(264kg) of CO_2 is generated by 1kmol of C_6H_6, the required work for liquefaction is 60.7MJ/kmol of C6H6 (3.9% of the work produced in the cycle)

Total sequestration work is 119.3MJ/kmol of C6H6 (7.6% of the work produced in the cycle)

(4) $\eta_{II} = \dfrac{Ideal\ work}{Actual\ work}$,

$Actual\ work = Ideal\ work / \eta_{II} = 1.25 \cdot Ideal\ work$

Hence, 25% increase of the sequestration work (149.1MJ/kmol of C6H6 and 9.5% of the work produced in the cycle.)

(5) Since no entropy should be generated in the process to minimize the required work, the temperature of the device should be regulated to be the same as that of environment (Isothermal compression). Note that work is supplied for separation and hence should be removed in the form of heat to the environment to keep the temperature constant. To reject heat while maintaining the temperature requires this process to occur very slowly.

(6) Instead of using isothermal compression, one can consider isentropic compression and heat rejection in a real situation. As we learned from problem II in Homework I, one can reduce the required work using intercooling. If one uses a large number of intercoolings and compressors, one can bring these compression and heat rejection processes closer to the ideal isothermal process. However, this will increase the capital cost of the plant. Using 3 compressors as shown below, the required work is 72.6MJ/kmol of C_6H_6 (20% increase over the isothermal work)

Figure 8.12b Temperature-entropy (T-S) diagram for pure CO_2 [provided by Professor Steven Penoncello, Center for Applied Thermodynamics Studies, University of Idaho, Moscow, Idaho].
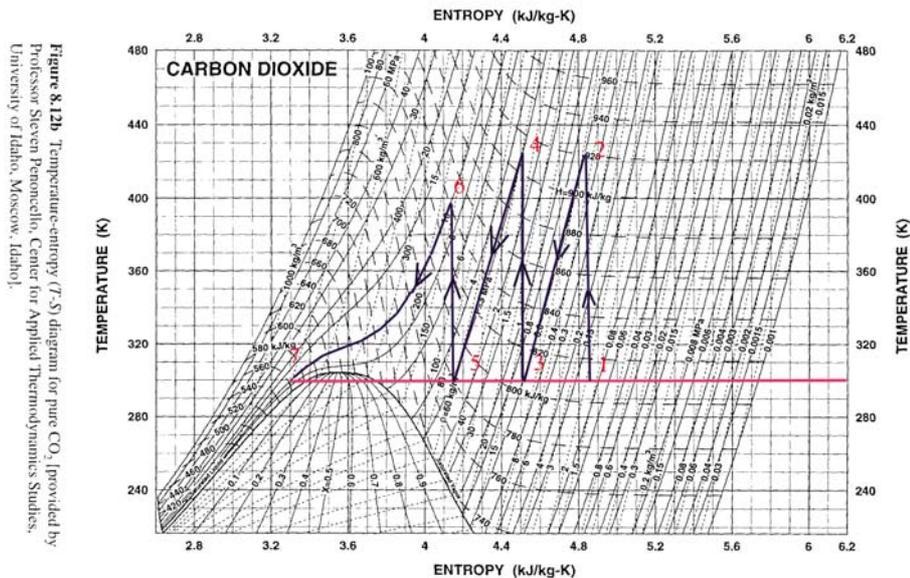
State 1
T1=300K, P1=1atm, h1=810kJ/kg

State 2 (Isentropic compression 1)
P2=6atm, S2=S1, h2=920kJ/kg

State 3 (heat rejection)
T3=300K, P3=6atm, h3=805kJ/kg

State 4 (Isentropic compression 2)
P4=30atm, S4=S3, h4=910kJ/kg

State 5 (heat rejection)
T5=300K, P5=30atm, h5=780kJ/kg

State 6 (Isentropic compression 3)
P6=100atm,S6=S5, h6=840kJ/kg

State 7 (heat rejection)
T7=300K, P7=100atm, h7=560kJ/kg

II.

In combustion process, this has only O_2 and C_6H_6 in the reactant:

$$C_6H_6 + XO_2 \rightarrow 6CO_2 + 3H_2O + (X - 7.5)O_2$$
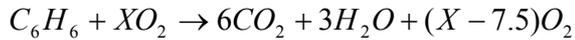
From $H_R(T_2 = 832K) = H_p(T_3 = 1573K)$, we get $X = 110.56$.

Hence, in the initial separation of N2

110.56*3.76N2+
110.56O2

T=300K,
P=1atm

110.56*3.76N2

110.56O2

T=300K,
P=1atm
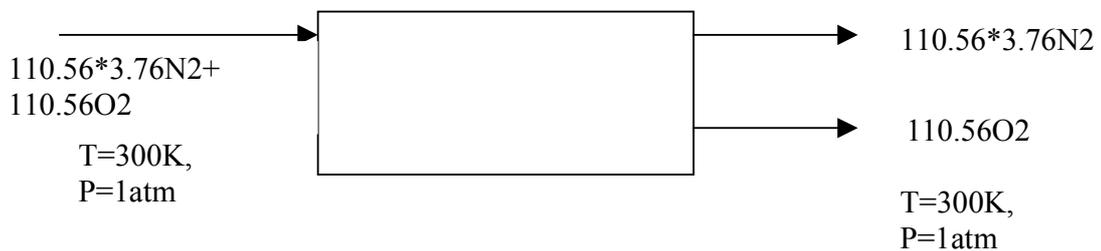
Required work for separation: 674.8MJ/kmol of C6H6 (Significant increase in work due to the increase in the number of moles being separated)

However, if we do not throw out O_2 after the turbine and circulate it, we only use 7.5moles of O_2 instead of 110.56moles per 1 mole of C6H6. Hence, the required work is
674.8MJ/kmol*7.5moles/110.56moles=45.8MJ/kmol of C6H6

One problem of circulating O_2 is that we need to separate O_2 from CO_2 in the product as follow:

6CO2+103.06O2

T=300K,
P=1atm

6CO2

103.06O2

T=300K,
P=1atm
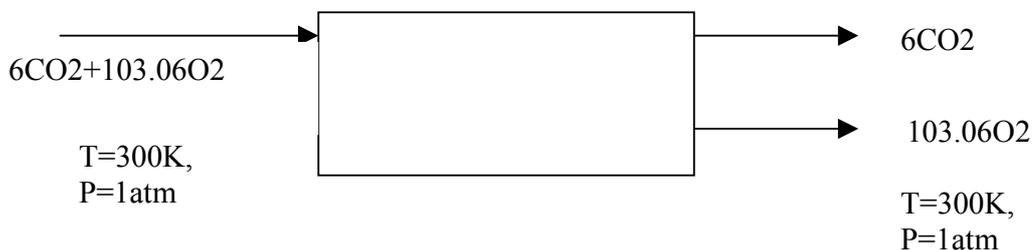
The required work of this process is 58.0MJ/kmol of C6H6.

Total required work for separation is 45.8+58=103.8MJ/kmol of C6H6.

There is no change in the liquefaction work of CO_2.

III.

Combustion (adiabatic, p=1atm)

$$C_6H_6 + 6(O_2 + 3.76N_2) \rightarrow 6CO_2 + 3H_2 + 6*3.76N_2$$
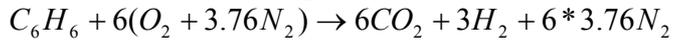
From $H_R(T_1 = 300K) = H_p(T_2)$, we get $T_2 = 2342\,K$

Separation (Const T)
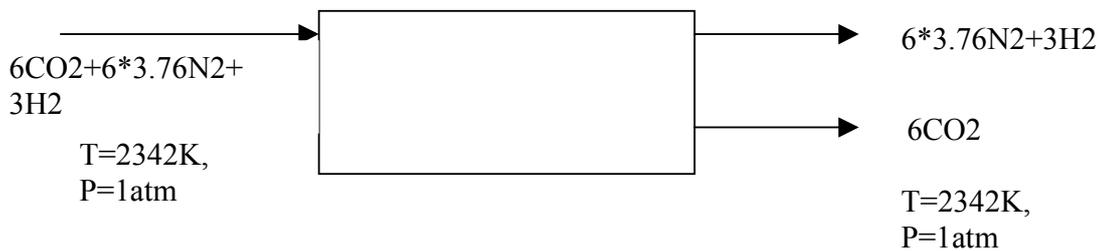
Required work for separation: 299MJ/kmol of C6H6 (Significant increase due to increase in T)

For the liquefaction work, if we assume inlet temperature is 300K, then we get the same required work (60.7MJ/kmol of C6H6). However, note that we may be able to use extracted heat from CO_2 since the temperature of the CO_2 after the separator is 2342K. The availability of CO_2 can be calculated in the following process, assuming environment temperature is 300K
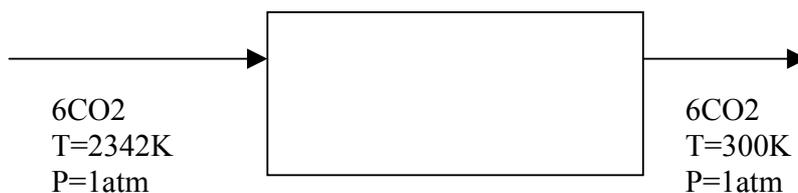
$$W_{max} = H_1 - H_2 - T_o(S_1 - S_2) = 6moles*(112MJ/kmol - 300K*0.319MJ/kmol)$$
$$= 97.8MJ$$

Hence, the total required work for sequestration is
(299-97.8+60.7)*MJ/kmol* of C6H6=262*MJ/kmol* of C6H6