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Thapar Institute of Engineering &  
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Course: Material and Energy Balances  
UCH301

Course Instructor:

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# SOLVING M.B.& E.B. Simultaneously

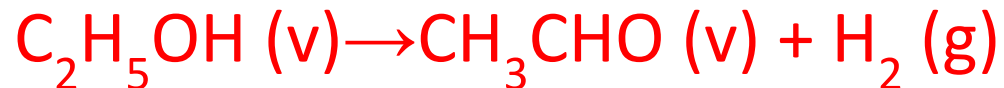


## Exercise

- The ethanol dehydrogenation to form acetaldehyde is carried out with the feed entering at 300 °C. The feed, 150 mol/s, contain 90 mol% ethanol and the balance acetaldehyde. To keep the reactor temperature from dropping too much heat is transferred to the reactor. When the heat addition is 2440 kJ/s, the outlet temperature is 253 °C.

**Calculate the fractional conversion of the ethanol.**

Reaction:



# Data

Std. heat of formation of ethanol(g)

$$\Delta H_{f, \text{CH}_3\text{OH (v)}}^0 = -235.31 \text{ kJ/mol}$$

- Std. heat of formation of Acetaldehyde(g)

$$\Delta H_{f, \text{CH}_3\text{CHO (v)}}^0 = -166.2 \text{ kJ/mol}$$

Std. heat of formation of hydrogen(g)

$$\Delta H_{f, \text{H}_2 \text{ (g)}}^0 = 0$$

$$C_p[\text{kJ}/(\text{mol} \cdot ^\circ\text{C})] \text{ or } [\text{kJ}/(\text{mol} \cdot \text{K})] = a + bT + cT^2 + dT^3$$

Hydrogen:  $a \times 10^3 = 28.84$ ;  $b \times 10^5 = 0.00765$ ;  $c \times 10^8 = 0.3288$ ;  $d \times 10^{12} = -0.8698$

Ethyl alcohol:  $a \times 10^3 = 61.34$ ;  $b \times 10^5 = 15.72$ ;  $c \times 10^8 = -8.749$ ;  $d \times 10^{12} = 19.83$

Acetaldehyde:  $a \times 10^3 = 50.48$ ;  $b \times 10^5 = 13.26$ ;  $c \times 10^8 = -8.050$ ;  $d \times 10^{12} = 23.80$





# Solution

- Feed = 150 mol/s
- Ethanol in feed =  $150 \times 0.9 = 135$  mol/s
- Acetaldehyde in feed =  $150 - 135 = 15$  mol/s

150 mol/s  
300 °C  
90% C<sub>2</sub>H<sub>5</sub>OH  
10% CH<sub>3</sub>CHO



n1 mol C<sub>2</sub>H<sub>5</sub>OH/s  
n2 mol CH<sub>3</sub>CHO/s  
n3 mol H<sub>2</sub>/s  
253 °C





- Calculate values of enthalpy from the Data:

$$H_i = \Delta H_{fi}^0 + \int_{25}^{T} C_{p,i} dT \quad (T \text{ from 25 to 300 for inlet and 25 to 253 for outlet})$$

$$H_i = \Delta H_{f,i} + \int_{25}^{300} C_{p,i} dT \quad \text{for input species}$$

$$H_i = \Delta H_{f,i} + \int_{25}^{253} C_{p,i} dT \quad \text{for output species}$$

Std. heat of formation of ethanol(g)

$$\Delta H_{f, \text{CH}_3\text{OH (v)}}^0 = -235.31 \text{ kJ/mol}$$

Std. heat of formation of Acetaldehyde(g)

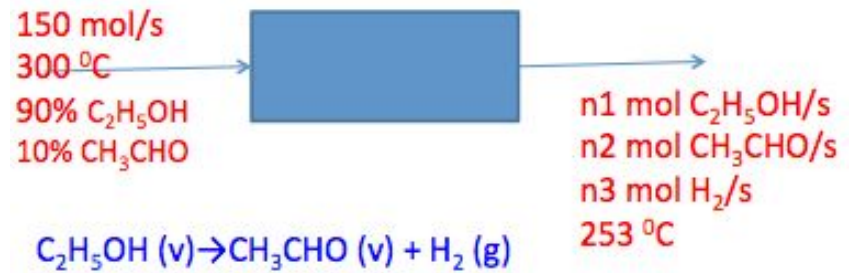
$$\Delta H_{f, \text{CH}_3\text{CHO (v)}}^0 = -166.2 \text{ kJ/mol}$$

Std. heat of formation of hydrogen(g)

$$\Delta H_{f, \text{H}_2 \text{ (g)}}^0 = 0$$

Substance	nin	Hin (kJ/mol)	nout	Hout (kJ/mol)
C <sub>2</sub> H <sub>5</sub> OH	135	-212.19	n1	-216.81
CH <sub>3</sub> CHO	15	-147.07	n2	-150.9
H <sub>2</sub>	-	-	n3	6.595





Since conversion is not given we will have solve Material and Energy balances simultaneously

- C balance:

$$135 \cdot 2 + 15 \cdot 2 = n_1 \cdot 2 + n_2 \cdot 2$$

➡ Or  $n_1 + n_2 = 150$

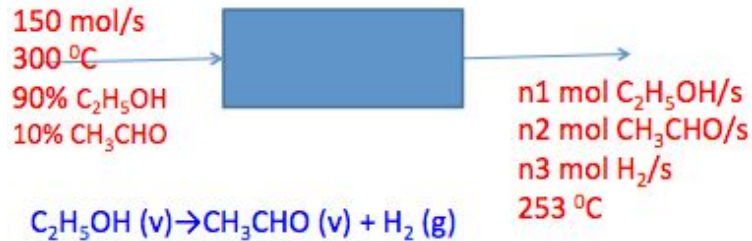
- H balance:

$$135 \cdot 6 + 15 \cdot 4 = 6n_1 + 4n_2 + 2n_3$$

➡  $3n_1 + 2n_2 + n_3 = 435$

Three unknowns  $n_1, n_2, n_3$ ; therefore one more equation from E.B. is required





Substance	n <sub>in</sub>	H <sub>in</sub> (kJ/mol)	n <sub>out</sub>	H <sub>out</sub> (kJ/mol)
C <sub>2</sub> H <sub>5</sub> OH	135	-212.19	n1	-216.81
CH <sub>3</sub> CHO	15	-147.07	n2	-150.9
H <sub>2</sub>	-	-	n3	6.595

From Energy Balance:

$$Q = \Delta H = \sum (n_i H_i)_{\text{outlet}} - \sum (n_i H_i)_{\text{inlet}}$$

$$2440 = \{-216.81 * n1 - 150.9 * n2 + 6.595 * n3\} - (135) * (-212.19) - (15) * (-147.07)$$

$$\text{Or } 216.81 n1 + 150.9 n2 - 6.595 n3 = 28412$$

The above equation and two m.b. equations can be solved simultaneously for n1, n2 and n3.







$$n_1 + n_2 = 150$$

$$3n_1 + 2n_2 + n_3 = 435$$

$$216.81 n_1 + 150.9 n_2 - 6.595 n_3 = 28412$$

**Solving three equations simultaneously**

$$n_1 = 91.95 \text{ mol/s}; n_2 = 58.04 \text{ mol/s}; n_3 = 43.05 \text{ mol/s}$$

$$X_{\text{ethanol}} = (\text{Ethanol in feed} - \text{Ethanol in product}) / (\text{Ethanol in feed})$$

$$\begin{aligned} \text{Fractional conv. of ethanol} &= (135 - 91.95) / 135 \\ &= 0.318 \end{aligned}$$





# Heating value of Fuel & Adiabatic Flame Temperature





- The heating value of a fuel is the negative of standard heat of combustion.
- The gross/high heating value is obtained if the water vapor formed are condensed.
- The net/lower heating value is obtained if the water vapor formed are not condensed
- Therefore, to determine the heating value, the moles of water vapor formed per mol of fuel burned are calculated
- If a fuel contains a mixture of combustible substances, its heating value is

$$H_v = \sum x_i (HV_i) \quad x_i \text{ is mass or mol fraction}$$





## Problem

- A natural gas contains 85% CH<sub>4</sub> and 15% C<sub>2</sub>H<sub>6</sub>. The heats of combustion of methane and ethane at 25 °C and 1 atm with water vapor as product are:

$$\Delta H^0_{C,CH_4} = -802 \text{ kJ/mol}; \Delta H^0_{C,C_2H_6} = -1428 \text{ kJ/mol}$$

Calculate Higher heating value (kJ/g) of the natural gas.

$$\Delta H_{v,H_2O} = 44.013 \text{ kJ/mol (at 25 °C)}$$





## SOLUTION

1 mol fuel contain 0.85 mol  $\text{CH}_4$  and 0.15 mol  $\text{C}_2\text{H}_6$ , that is 13.6 g  $\text{CH}_4$  and 4.5 g  $\text{C}_2\text{H}_6$

Total weight of fuel = 18.1 g

$$x_{\text{CH}_4} = 13.6/18.1 = 0.751; x_{\text{C}_2\text{H}_6} = 0.249$$



$$(\text{HHV})_{\text{CH}_4} = \text{LHV} + n_{\text{H}_2\text{O}} (\Delta H_v)_{\text{H}_2\text{O}}$$

$$(\Delta H_v)_{\text{H}_2\text{O}} = 44.013 \text{ KJ/mol (at } 25^\circ\text{C)}$$

$$\begin{aligned}(\text{HHV})_{\text{CH}_4} &= [802 \text{ kJ/mol} + (2\text{mol H}_2\text{O/mol CH}_4) \\ &\quad * 44.013 \text{ kJ/mol H}_2\text{O}] / 16 = 55.6 \text{ kJ/g}\end{aligned}$$

$$\begin{aligned}(\text{HHV})_{\text{C}_2\text{H}_6} &= [1428 \text{ kJ/mol} + (3\text{mol H}_2\text{O/mol C}_2\text{H}_6) \\ &\quad * 44.013 \text{ kJ/mol H}_2\text{O}] / 30 = 52.0 \text{ kJ/g}\end{aligned}$$

$$(\text{HHV})_{\text{mix}} = 0.751 * 55.6 + 0.249 * 52 = 54.7 \text{ kJ/g}$$





# Adiabatic flame temperature

- The highest achievable temperature reached if the reactor is adiabatic and all of the energy released by the combustion goes to raise the temperature of the combustion products. This temperature is called the **adiabatic flame temperature,  $T_{ad}$** .

