

ChE M1B Paper 1: January 1996

- 1 b). A supply of fuel has the following composition, in mass %: carbon = 72.0, hydrogen = 4.5, oxygen = 6.2, sulphur = 2.8, moisture = 7.5 and ash (non-combustibles) = 7.0. After combustion, the orsat analysis (dry basis) of the exhaust gas, in volume %, is as follows: (CO₂ + SO₂) = 12.2, CO = 1.0, O₂ = 6.6 and N₂ = 80.2. Assuming that the air supply contained no water vapour in it and that all the carbon, hydrogen, oxygen and sulphur take part in the combustion reaction calculate,
- the percentage excess air used
 - the complete combustion of the exhaust gas in mole %, including the water vapour
 - the temperature of the exhaust gas at which condensation of water begins, if the total pressure is 1.03 bar.
- DATA: Air contains 21 % oxygen and 79 % nitrogen by volume. The relative atomic masses are C = 12.0, H = 1.0, O = 16.0, N = 14.0 and S = 32.0. The relationship between the vapour pressure of water (p_w^o in bar) and absolute temperature (T in K) is, $\{ \ln p_w^o = 14.2517 - 5280 / T \}$, where \ln is the logarithm to the base e .

Solution:

(i) Percentage excess air

BASIS = 100 moles of dry exhaust gas

There is no nitrogen in the fuel, so all the N₂ in the dry flue gas must have come from the air supplied

Therefore, the amount of O₂ accompanying this nitrogen at inlet = $(80.2 / 79) \times 21 = 21.32$ moles

Oxygen in the dry flue gas is NOT the excess O₂ since there is some CO in the dry flue gas.

Therefore, excess oxygen = O₂ in dry flue gas - O₂ required to oxidise CO to CO₂ = $6.6 - 1.0 / 2 = 6.1$ moles

Theoretical O₂ = Oxygen supplied - excess oxygen = $21.32 - 6.1 = 15.22$ moles.

% excess O₂ = % excess air = $\{ (\text{Excess} / \text{Theoretical}) \times 100 \} = \{ (6.1 / 15.22) \times 100 = 40\%$

(ii) Complete composition of the exhaust gas

BASIS = 100 moles of dry exhaust gas

Need to calculate the amount of water produced during combustion

Since the fuel is completely burnt, the ratio of $\{ \text{H}_2 / (\text{C} + \text{S}) \}$ in the fuel = the ratio of $\{ \text{H}_2 \text{ as moisture} / (\text{C} + \text{S}) \}$ in the flue gas

In 100 kg of fuel,

Carbon = 72 kg = 6.0 kmols

Sulphur = 2.8 kg = 0.0875 kmols

Hydrogen = 4.5 kg = 2.25 kmols

H₂ in moisture = 7.5 kg = 0.4167 kmols

the ratio of $\{ \text{H}_2 / (\text{C} + \text{S}) \}$ in the fuel = $\{ (2.25 + 0.4167) / (6.0 + 0.875) \} = 0.4381$

= the ratio of $\{ \text{H}_2 \text{ as moisture} / (\text{C} + \text{S}) \}$ in the flue gas = $\{ \text{H}_2 \text{ as moisture} / (\text{C in CO}_2 + \text{C in CO} + \text{S in SO}_2) \} = \text{H}_2 \text{ as moisture} / (12.2 + 1.0)$

Therefore, = H₂ as moisture = $(12.2 + 1.0) \times 0.4167 = 5.78$ kmols

Composition of the exhaust gas

CO ₂ + SO ₂	=	12.2	=	11.53%
CO	=	1.0	=	0.95%
O ₂	=	6.6	=	6.24%
N ₂	=	80.2	=	75.82%
Moisture	=	5.78	=	5.46%
Total	=	105.78		

(iii) Condensation temperature

Water will start to condense when the partial pressure of water vapour is equal to its vapour pressure

Partial pressure = mole fraction \times total pressure = $\{ (5.46 / 100) \times 1.03 = 0.05624$ bar

Given that $\{ \ln p_w^o = 14.2517 - 5280 / T \}$,

T = $\{ 5280 / (14.2517 - \ln(0.05624)) \} = 308 \text{ K} = 35^\circ\text{C}$

ChE M1R Paper 1: January 1997

1 (b). A boiler is fired with coal which has the following composition, in mass %: carbon = 76.9, hydrogen = 3.8, nitrogen = 1.4, sulphur = 0.8, oxygen = 1.6, moisture = 9.0 and ash = 6.5. Assume that the air supply to the burner is dry and that all the carbon, hydrogen, oxygen and sulphur take part in the combustion reaction.

- i) Calculate, the theoretical air required for the complete combustion in kg of air per kg of coal burned
- ii) If 30 % excess air is used and 10 mass % of the carbon forms carbon monoxide, what would be the Orsat analysis of the gases leaving the burner ?
- iii) What would be the temperature of the gas at which condensation of water begins for the incomplete combustion, if the total pressure is 1.03 bar ?

DATA: Air contains 21 % oxygen and 79 % nitrogen by volume. The relative atomic masses are C = 12.0, H = 1.0, O = 16.0, N = 14.0 and S = 32.0. The relationship between the vapour pressure of water (p_w^o in bar) and absolute temperature (T in K) is, $\{ \ln p_w^o = 14.2517 - 5280 / T \}$, where \ln is the logarithm to the base e .

Solution:

BASIS = 100 kg of fuel

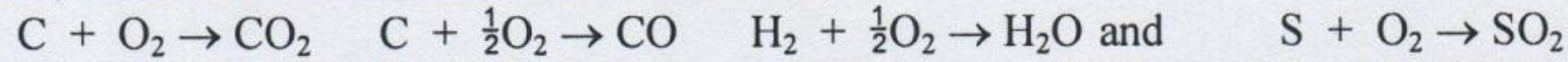
The reactions for complete combustion are, $C + O_2 \rightarrow CO_2$ $H_2 + \frac{1}{2}O_2 \rightarrow H_2O$ and $S + O_2 \rightarrow SO_2$

Component	mass %	kg	RMM	kmoles	Theoretical O ₂ required
Carbon	76.9	76.9	12	6.41	6.41 kmoles
Hydrogen	3.8	3.8	2	1.90	0.95 kmoles
Nitrogen	1.4	1.4	28	0.05	-
Sulphur	0.8	0.8	32	0.025	0.025 kmoles
Oxygen	1.6	1.6	32	0.05	- 0.05 kmoles
Moisture	9.0	9.0	18	0.50	
Ash	6.5	6.5			
Total	100				7.335 kmoles

Air contains 21 % oxygen

∴ theoretical air required = $(7.335 / 21) \times 100 = 34.93$ kmoles = 1012.97 kg of air per 100 kg of coal. ie. = **10.13 kg of air per kg of coal.**

(ii) During incomplete combustion, when CO is also formed the reactions are,



Given that 10 % of C forms CO and 90 % of C forms CO₂ ie 5.769 kmoles of C forms CO₂ and 0.641 kmoles of C forms CO

Air supplied = 30 % excess = $34.93 \times 1.30 = 45.409$ kmoles

21 % is oxygen = $0.21 \times 45.409 = 9.54$ kmoles and 79 % is nitrogen = $0.79 \times 45.409 = 35.87$ kmoles

Component	O ₂ used
Carbon to CO ₂	5.769 kmoles
Carbon to CO	$(0.641 / 2) = 0.3205$ kmoles
Hydrogen to Water vapour	0.95 kmoles
Nitrogen	-
Sulphur to SO ₂	0.025 kmoles
Oxygen	- 0.05 kmoles
Total	7.015 kmoles

Orsat analysis

Component	kmoles	mole %
(CO ₂ + SO ₂)	5.794	12.91
Carbon monoxide	0.641	1.43
Nitrogen	$(35.87 + 0.05) = 35.92$	80.03
Oxygen	$(9.54 - 7.015) = 2.526$	5.63
Total	44.881	100

(ii) Water will start to condense when the partial pressure = vapour pressure

Total water in product = water in fuel + water formed during combustion = $0.5 + 1.9 = 2.4$ kmoles

Total of flue gas including water = $(44.881 + 2.4) = 47.281$

partial pressure = mole fraction \times total pressure = vapour pressure, $p_w^o = (2.4 / 47.281) \times 1.03 = 0.0523$ bar

$$\{ \ln p_w^o = 14.2517 - 5280 / T \} \ln (0.0523) = -2.9508 = 14.2517 - 5280 / T. \text{ from which } T = 307 \text{ K} = 34^\circ \text{ C}$$

Q2 (a) May/June 1993 - ChE 1A2

A gas stream has the following composition, in mole %: CO = 16.0, CO₂ = 20.0, H₂ = 20.0, Water (vapour) = 44.0. To make this gas suitable for a hydrocarbon synthesis, the ratio of H₂ to CO (in moles) has to be changed to 3 to 1. To do this, the stream is passed through an adiabatic reactor in which the gas phase reaction CO + H₂O → CO₂ + H₂ occurs. The reaction can be assumed to proceed to equilibrium at 1 atmosphere pressure and perfect gas behaviour can be assumed.

- (i) What will be the outlet temperature from the reactor ?
- (ii) What should be the temperature of the gas stream entering the reactor ?

DATA: For the reaction CO + H₂O → CO₂ + H₂ the relationship between the equilibrium constant (K) and absolute temperature (T, in K) for a standard state pressure of 1 atmosphere is $\ln K = (4519 / T) - 4.268$ where ln is the logarithm to the base e. The standard state enthalpy change for the reaction at 298 K is -38,000 kJ/kmol. The mean specific heat capacities (c_p) for the temperature range involved are as follows (in kJ (kmol K)⁻¹): CO = 33, CO₂ = 46, H₂ = 27 and H₂O = 40.

SOLUTION:

BASIS = 100 mols of gas stream entering the reactor.

The reaction is CO + H₂O → CO₂ + H₂

Limiting reactant for the process is CO as it will be used up first

Let X mols of CO reacts in the reactor.

Amount of CO in the products = (16 - X) mols

Amount of H₂ in the products = (20 + X) mols

$$\frac{H_2}{CO} = \frac{3.0}{1.0} = \frac{(20 + X)}{(16 - X)} \text{ from which, } X = 7.0 \text{ mols.}$$

Composition of reactor products:

CO = (16 - 7) = 9.0 mols

H₂O = (44 - 7) = 37 mols

H₂ = (20 + 7) = 27 mols

CO₂ = (20 + 7) = 27 mols

Total number of moles = 100

$$K = \frac{P_{CO_2} \times P_{H_2}}{P_{CO} \times P_{H_2O}} = \frac{y_{CO_2} \times y_{H_2}}{y_{CO} \times y_{H_2O}} \times P = \frac{0.27 \times 0.27}{0.09 \times 0.37} \times 1.0 = 2.189$$

$$\ln K = \ln(2.189) = 0.7835 = (4519 / T) - 4.268$$

From which T = 894.6 K.

The temperature of products leaving the reactor = 894.6 K

For an adiabatic reactor

$$\Delta H = 0 = \Delta H_{Ti} + \Delta H_r + \Delta H_{T1}$$

-38000 kJ/kmol

Assuming 298K as the reference temperature,

$$\begin{aligned} \Delta H_{Ti} &= \{(n_{CO} c_p CO) + (n_{H_2} c_p H_2) + (n_{H_2O} c_p H_2O) + (n_{CO_2} c_p CO_2)\} \times (298 - T_i) \text{ kJ} \\ &= \{(16 \times 33) + (20 \times 27) + (44 \times 40) + (20 \times 46)\} \times (298 - T_i) \text{ kJ} \\ &= (1116904 - 3748 T_i) \text{ kJ} \end{aligned}$$

Standard enthalpy of reaction is -38000 kJ/kmol

$$\Delta H_{Tr} = 7 \times -89700 = -266000 \text{ kJ}$$

$$\Delta H_{T1} = \Sigma(m c_p) dT$$

$$\begin{aligned} \Delta H_{T1} &= \{(n_{CO} c_p CO) + (n_{H_2} c_p H_2) + (n_{H_2O} c_p H_2O) + (n_{CO_2} c_p CO_2)\} \times (T_1 - 298) \text{ kJ} \\ &= \{(9 \times 33) + (27 \times 27) + (37 \times 40) + (27 \times 46)\} \times (894.6 - 298) \text{ kJ} \\ &= 2236056.8 \text{ kJ} \end{aligned}$$

$$\Delta H = 0 = (1116904 - 3748 T_i) + (-266000) + (2236056.8)$$

From which, T₁ = 823.6 K

The inlet temperature of the feed to the reactor = 823.6 K

Q1 (a) May/June 1998 - ChE M1R Paper 2

(Graph paper required)

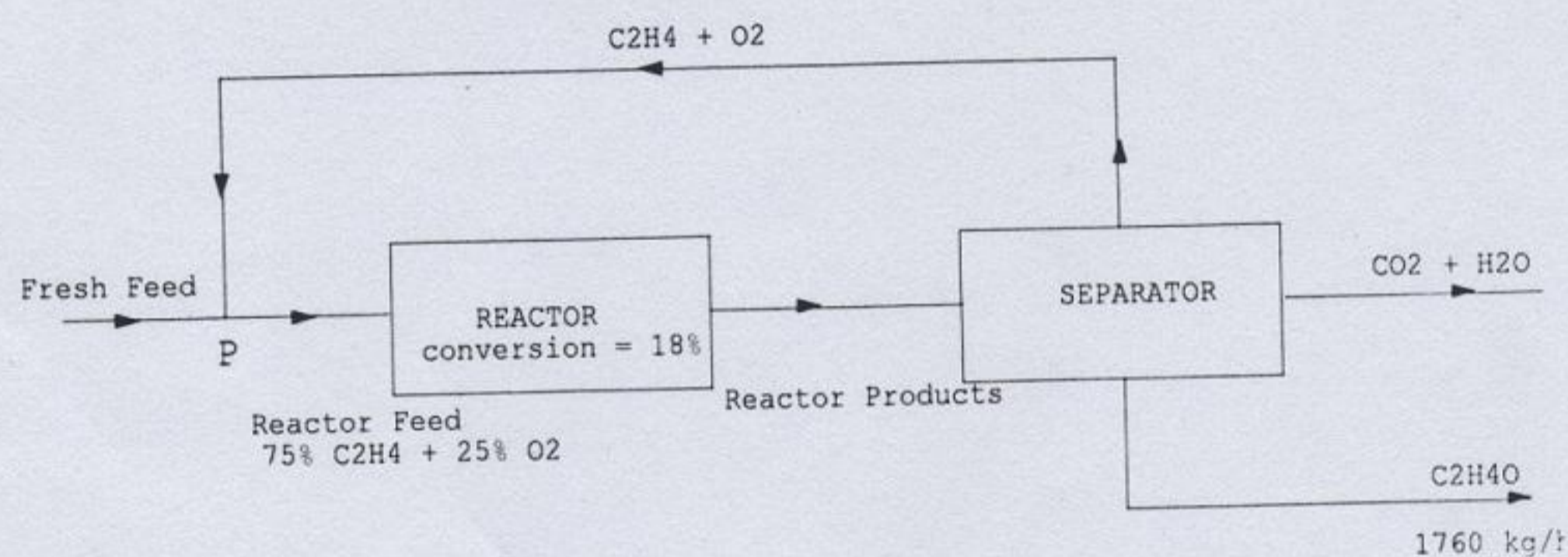
A fresh feed containing ethylene and oxygen is used to produce ethylene oxide by the reaction, $2C_2H_4 + O_2 \rightarrow 2C_2H_4O$. The most important side reaction that can occur in the reactor is the complete oxidation of ethylene as follows, $C_2H_4 + O_2 \rightarrow 2CO_2 + H_2O$. The product stream from the reactor is then passed through a series of separation units where all the C_2H_4O is recovered and all the CO_2 and H_2O are removed. All the unreacted ethylene and oxygen are recycled back to the reactor after mixing with the fresh feed. The feed to the reactor (not the fresh feed) contains 75 mole % ethylene and 25 mole % oxygen. If the single pass conversion of ethylene in the reactor is 18 % and, only 85 % of the C_2H_4 that reacts in the reactor forms C_2H_4O , calculate,

- (i) the composition in mole % of the reactor products (12 marks)
 (ii) the mass flow rates of C_2H_4 and O_2 in the fresh feed that are required to produce 1760 kg/h of ethylene oxide. (9 marks)

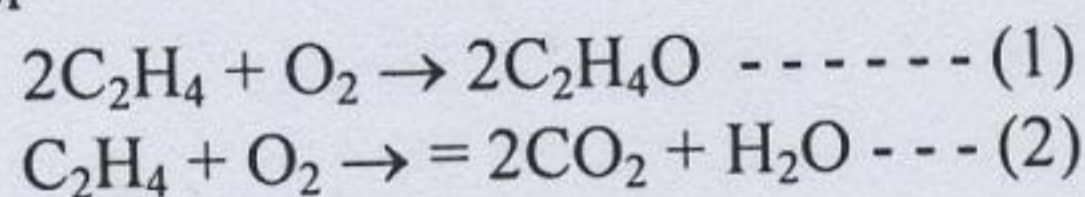
The relative atomic masses are C = 12, H = 1 and O = 16

(Hint: Use 100 kmols of feed to the reactor as the basis for your calculation to find the composition of the reactor products. Carry out material balance at mixing point to obtain the composition of the fresh feed. Scale-up for the required amount of product)

SOLUTION.



BASIS = 100 kmols of feed to the reactor



- (i) Reactor products:
 Total amount of ethylene reacted = $0.18 \times 75 = 13.5$ kmols of which 85% is used for reaction (1)
 Unreacted ethylene = $(1.0 - 0.18) \times 75 = 61.5$ kmols
 Amount of ethylene used for reaction (1) = $0.85 \times 13.5 = 11.475$ kmols and,
 The amount of ethylene used for reaction (2) = $0.15 \times 13.5 = 2.025$ kmols

Oxygen balance: O_2 in product stream	= O_2 supplied - O_2 used in reactions (1) and (2)	
	= $25 - \{(\frac{1}{2} \times 11.475) + (3 \times 2.025)\}$	
	= $25 - 11.8125 = 13.188$ kmols	(13.99%)
Amount of CO_2 produced	= $2 \times 2.025 = 4.05$ kmols	(4.30%)
Amount of H_2O produced	= $2 \times 2.020 = 4.05$ kmols	(4.30%)
Amount of C_2H_4O produced	= $1 \times 11.475 = 11.475$ kmols	(12.17%)
Amount of unreacted ethylene	= 61.5 kmols	(65.24%)
TOTAL	= 94.263 kmols	

- (ii) Mass % of fresh feed
 Apply material balance at mixing point:
 (a) O_2 in Reactor feed = O_2 in fresh feed + O_2 in the recycle
 O_2 in the reactor feed = 25 kmols (from the basis for calculation)
 O_2 in the recycle = 13.188 kmols (from part (i))
 Therefore, O_2 in the Fresh Feed = $25 - 13.188 = 11.812$ kmols (= 378 kg)
 (b) C_2H_4 in Reactor feed = C_2H_4 in fresh feed + C_2H_4 in the recycle
 C_2H_4 in Fresh Feed = $75 - 61.5 = 13.5$ kmols (= 378 kg)
 Amount of C_2H_4O produced = 11.475 kmols (= 504.9 kg)

Therefore to produce 1760 kg/h of C_2H_4O , the amounts required are, by ratios,
 $O_2 = (378 / 504.9) \times 1760 = 1317.6$ kg