

Chemical Process Calculations CL204
Module-4
Material Balance With Chemical Reaction

Tutorials

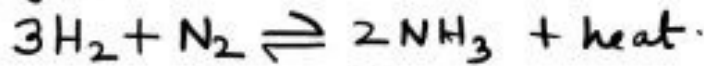
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Module - 1

Material balance with chemical reaction

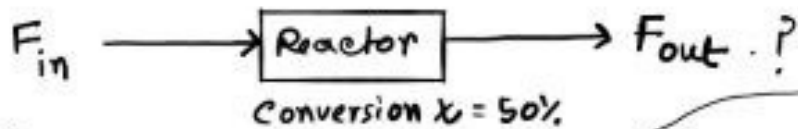
First consider a single reaction in a reactor block.

inert gas Argon
in other feed



$\Delta_r U^\circ$: -3 -1 +2 Exothermic reversible reaction.

$\Delta_r U_{\text{Argon}} = 0$



$F_{out}^{\text{N}_2} = 4.5 \text{ kmol/hr}$
 $F_{out}^{\text{H}_2} = 4.5 \text{ ''}$
 $F_{out}^{\text{NH}_3} = 3 \text{ kmol/hr}$
for 100% conversion

$$F_{in}^{\text{N}_2} = 6 \text{ kmol/hr}$$

$$F_{in}^{\text{H}_2} = 9 \text{ kmol/hr}$$

$$F_{in} = 6 + 9 = 15 \text{ kmol/hr}$$

1 mol of N_2 reacted with 3 mol of H_2
6 " " " " " " $\frac{3}{1} \times 6 = 18 \text{ mol of H}_2$
6 kmol/hr " " " " 18 kmol/hr of H_2

but H_2 inlet flowrate is 9 kmol/hr
So, H_2 is limiting reactant.

3 kmol/hr H_2
9 " " "
↓
Limiting

1 kmol/hr N_2 .
 $\frac{1}{3} \times 9 = 3$ kmol/hr
 N_2
excess.

So 50% conversion will be based on limiting reactant H_2 .

$$F_{in}^{H_2} = 6 \text{ kmol/hr.}$$

50% conversion, $9 \times 0.5 = 4.5$ kmol/hr H_2 will be reacted.

So outlet flowrate of H_2 , $F_{out}^{H_2} = 9 - 4.5 = 4.5$ kmol/hr

For N_2 , reacted = $4.5/3 = 1.5$ kmol/hr

$$\text{So } F_{out}^{N_2} = 6 - 1.5 = 4.5 \text{ kmol/hr}$$

$$\begin{aligned} NH_3 \text{ Formed} &= N_2 \text{ reacted} \times 2 \\ &= 1.5 \times 2 = 3 \text{ kmol/hr} \\ &= H_2 \text{ reacted} \times \frac{2}{3} \\ &= 4.5 \times \frac{2}{3} = \underline{3 \text{ kmol/hr}} \end{aligned}$$

excess $N_2 = 6 - 3 = 3$ kmol/hr N_2 .

$$\% \text{ excess} = \frac{6-3}{3} \times 100$$

$$= \underline{\underline{100\% \text{ excess } N_2}}$$

Generalized material balance for a reactor

$$F_i^{\text{out}} = F_i^{\text{in}} + \underline{v_i \xi}$$

$v_i \xi =$ molar flow change due to chemical reaction of species i

$\xi =$ extent of reaction

$$\xi = \frac{F_{\text{N}_2}^{\text{out}} - F_{\text{N}_2}^{\text{in}}}{v_{\text{N}_2}} = \frac{4.5 - 6}{-1} = 1.5 \quad \left[\xi = \frac{F_i^{\text{out}} - F_i^{\text{in}}}{v_i} \right]$$

$$\xi = \frac{F_{\text{H}_2}^{\text{out}} - F_{\text{H}_2}^{\text{in}}}{v_{\text{H}_2}} = \frac{4.5 - 9}{-3} = 1.5$$

$$\xi = \frac{F_{\text{NH}_3}^{\text{out}} - F_{\text{NH}_3}^{\text{in}}}{v_{\text{NH}_3}} = \frac{3 - 0}{2} = 1.5$$

$$\therefore F_i^{out} = F_i^{in} + \nu_i \xi$$

$$N_2: F_{N_2}^{out} = 6 + (-1) \times 1.5 = 4.5$$

$$H_2: F_{H_2}^{out} = 9 + (-3) \times 1.5 = 4.5$$

$$N_2: F_{N_2}^{out} = 0 + (2) \times 1.5 = 3$$

$$\xi = \frac{F_i^{out} - F_i^{in}}{\nu_i}$$

$$= - \left[\frac{(F_i^{in} - F_i^{out})}{F_i^{in}} \right] \frac{F_i^{in}}{\nu_i}$$

$$i = \text{Limiting reactant}; H_2 \rightarrow \frac{9 - 4.5}{9} = 0.5 = \underline{\underline{50\%}}$$

$$\frac{F_{LR}^{in} - F_{LR}^{out}}{F_{LR}^{in}} = X = \text{fractional conversion.}$$

$$\xi = -X \frac{F_{LR}^{in}}{\nu_{LR}}$$

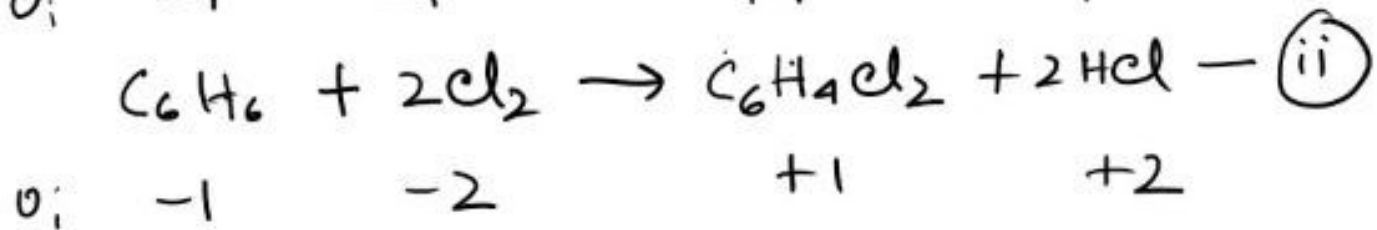
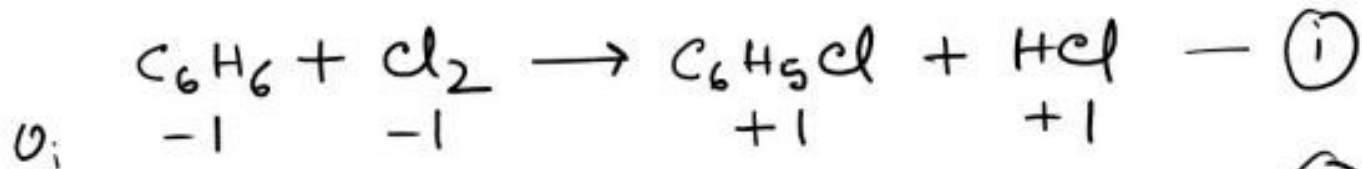
$$X = -\frac{\xi \nu_{LR}}{F_{LR}^{in}}$$

LR = Limiting reactant

$$\xi = -0.5 \frac{9}{(-3)}$$

$$\xi = 1.5$$

Material balance for multiple reaction



1st reaction extent of reaction ξ_1 .

2nd " " " " " ξ_2

Flowrate of benzene C_6H_6 in the inlet (reactor)
(Fresh feed + Recycle) = 100 kmol/hr.

Flowrate of Chlorine in the inlet (Reactor)
(Fresh feed + Recycle) = 111.11 kmol/hr.

in overall 2 mol C_6H_6 reacted with 3 mol Cl_2
100 " " " " " $\frac{3}{2} \times 100$
= 150 mol Cl_2

but feed flowrate Cl_2 is 111.11 kmol/hr

so, Cl_2 is limiting reactant

so, Benzene is excess reactant.

So, 111.11 kmol/hr Cl_2 will be reacted with.

$$= 111.11 \times \frac{2}{3} \text{ kmol/hr Benzene}$$

(100% conversion)

$$= 74.07 \text{ kmol/hr BZ.}$$

But overall conversion of benzene is 55.3% (given)

$$\therefore \text{converted benzene flowrate} = 100 \times \frac{55.3}{100}$$
$$= 55.3 \text{ kmol/hr.}$$

Product Stream having Bz flowrate
Unreacted Bz = $100 - 55.3 = 44.7 \text{ kmol/hr}$.

\therefore Overall Cl_2 conversion = $55.3 \times \frac{3}{2}$
= 82.95 kmol/hr .

\therefore Product Stream having Cl_2 = $111.11 - 82.95$
unreacted Cl_2 = 28.16 kmol/hr .

Monochlorobenzene $\text{C}_6\text{H}_5\text{Cl}$ in outlet.

$$= 55.3 \times \frac{1}{2} = 82.95 \times \frac{1}{3}$$

$$= 27.65 \text{ kmol/hr}$$

Dichlorobenzene, $\text{C}_6\text{H}_4\text{Cl}_2$ in reactor

$$\text{outlet} = 55.3 \times \frac{1}{2} = 82.95 \times \frac{1}{3}$$

$$= 27.65 \text{ kmol/hr}$$



$$\therefore x_{Bz}^{in} = \frac{100}{111.11 + 100}$$

$$\therefore x_{Cl_2}^{in} = \frac{111.11}{111.11 + 100}$$

$$F_{Cl_2}^{out} = 28.16 \text{ kmol/hr}$$

$$F_{Bz}^{out} = 44.7 "$$

$$F_{Mcl}^{out} = 27.65 "$$

$$F_{DCl}^{out} = 27.65 "$$

$$F_{HCl}^{out} = \frac{27.65}{\textcircled{i}} + \frac{2 \times 27.65}{\textcircled{ii}}$$

$$= 82.95 \text{ kmol/hr.}$$

$$x_{Cl_2}^{out} = \frac{F_{Cl_2}^{out}}{\sum F_i^{out}}$$

$$x_{Bz}^{out} = \frac{F_{Bz}^{out}}{\sum F_i^{out}}$$

$$x_{Mcl}^{out} = x_{DCl}^{out} =$$

Generalized material balance equations.

$$Bz: F_{Bz}^{out} = F_{Bz}^{in} + \xi_1 \nu_{Bz}^1 + \xi_2 \nu_{Bz}^2 \quad \textcircled{i}$$

$$\nu_{Bz}^1 = -1; \nu_{Bz}^2 = -1$$

$$Cl_2: F_{Cl_2}^{out} = F_{Cl_2}^{in} + \xi_1 \nu_{Cl_2}^1 + \xi_2 \nu_{Cl_2}^2 \quad \textcircled{ii}$$

$$\nu_{Cl_2}^1 = -1; \nu_{Cl_2}^2 = -2$$

$$\text{MCBZ: } F_{\text{MCBZ}}^{\text{out}} = F_{\text{MCBZ}}^{\text{in}} + \xi_1 \mathcal{U}_{\text{MCBZ}}^1 - \text{(iii)}$$

$$\mathcal{U}_{\text{MCBZ}}^2 = 0; \mathcal{U}_{\text{MCBZ}}^1 = +1.$$

$$\text{DCBZ: } F_{\text{DCBZ}}^{\text{out}} = F_{\text{DCBZ}}^{\text{in}} + \xi_2 \mathcal{U}_{\text{DCBZ}}^2 - \text{(iv)}$$

$$\mathcal{U}_{\text{DCBZ}}^1 = 0; \mathcal{U}_{\text{DCBZ}}^2 = +1$$

$$\text{HCl: } F_{\text{HCl}}^{\text{out}} = F_{\text{HCl}}^{\text{in}} + \xi_1 \mathcal{U}_{\text{HCl}}^1 + \xi_2 \mathcal{U}_{\text{HCl}}^2 - \text{(v)}$$

$$\mathcal{U}_{\text{HCl}}^1 = +1; \mathcal{U}_{\text{HCl}}^2 = +2.$$

$$f(\text{conversion}) = f(\xi_1, \xi_2).$$

If overall conversion of Bz is x_{Bz}
 " " " " Cl₂ " x_{Cl_2}

$$\Rightarrow \frac{-\mathcal{U}_{\text{Bz}}^1 \xi_1 - \mathcal{U}_{\text{Bz}}^2 \xi_2}{F_{\text{Bz}}^{\text{in}}} = x_{\text{Bz}} - \text{(vi)}$$

$$\Rightarrow \frac{-\mathcal{U}_{\text{Cl}_2}^1 \xi_1 - \mathcal{U}_{\text{Cl}_2}^2 \xi_2}{F_{\text{Cl}_2}^{\text{in}}} = x_{\text{Cl}_2} - \text{(vii)}$$

Say yield of MCBZ is 27.65% } \Rightarrow given.
Yield of DCBZ is 27.65% } or kmol

Yield is in the form of kmol/hr of a product
Formed Per kmol/hr of Benzene in the feed.
or kmol.

$$\begin{aligned}\text{Yield of MCBZ} &= \frac{27.65 \text{ kmol/hr}}{100 \text{ kmol/hr}} \\ &= 0.2765 \\ &= 27.65\%\end{aligned}$$

$$\text{Yield of DCBZ} = 27.65\%$$

$$\begin{aligned}\underline{\text{MCBZ}}: \xi_1 &= \frac{F_{\text{MCBZ}}^{\text{out}} - F_{\text{MCBZ}}^{\text{in}}}{\theta_{\text{MCBZ}}^1} \\ &= \frac{27.65 - 0}{+1} = 27.65\end{aligned}$$

$$\begin{aligned}\text{DCBZ}: \xi_2 &= \frac{27.65 - 0}{+1} = 27.65 \\ \Rightarrow \xi_1 &= \xi_2 = 27.65\end{aligned}$$

Put in the (i)

$$\begin{aligned}\text{BZ}: F_{\text{BZ}}^{\text{out}} &= 100 + 27.65 \times (-1) + 27.65 \times (-1) \\ F_{\text{BZ}}^{\text{out}} &= 44.7 \text{ kmol/hr (checked)}\end{aligned}$$

$$\text{Cl}_2: F_{\text{Cl}_2}^{\text{out}} = 111.11 + 27.65 \times (-1) + 27.65 \times (-2)$$

$$F_{\text{Cl}_2}^{\text{out}} = 28.16 \text{ kmol/hr (checked)} \checkmark$$

$$\text{mCBZ}: F_{\text{mCBZ}}^{\text{out}} = 0 + 27.65 \times (+1)$$

$$= 27.65 \text{ kmol/hr (checked)} \checkmark$$

$$\text{DcBZ}: F_{\text{DcBZ}}^{\text{out}} = 0 + 27.65 \times (+1)$$

$$= 27.65 \text{ kmol/hr (checked)} \checkmark$$

$$\text{Cl}_2: F_{\text{HCl}}^{\text{out}} = 0 + 27.65 \times (+1) + 27.65 \times (+2)$$

$$= 82.95 \text{ kmol/hr (checked)} \checkmark$$

If conversion of products are given.

Find (calculate) ξ_1 & ξ_2 from equation (vi) & (vii) [solve ξ_1 & ξ_2]

And calculate outlet concentration from material balance equations.

Yield is given 30%. $\left(\frac{\text{kmol of product}^{\text{produced}}}{\text{kmol of B}_2 \text{ reacted}} \times 100 \right)$

$$\therefore 0.3 = \frac{F_{\text{mCBZ}}^{\text{produced}}}{55.3}$$

$$\Rightarrow F_{\text{mCBZ}}^{\text{produced}} = 0.3 \times 55.3 \text{ kmol/hr}$$

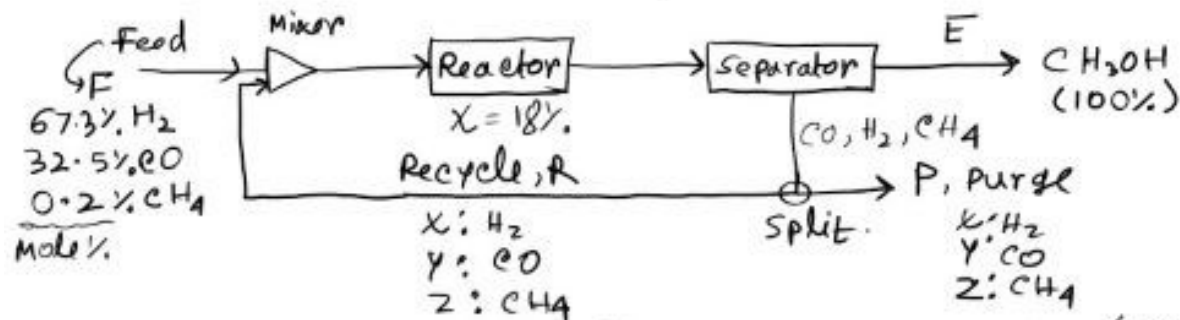
$$= 16.59 \text{ kmol/hr}$$

$$F_{\text{mCBZ}}^{\text{out}} = \underline{\underline{16.59 \text{ kmol/hr}}}$$

Material balance of system with reactor, separator mixer, and with recycle and purging streams.

↳ Material balance with chemical reaction in a chemical process.
like, production of NH_3 , $\text{C}_2\text{H}_4\text{Cl}_2$,
 MCB_2 , DCB_2 , etc.

Consider a steady state open process where the following reaction takes place:



x, y, z are mole fraction $z = 0.032 (\text{CH}_4) \cdot (3.2 \%)$.

$$\nu_{\text{CO}} = -1 ; \quad \nu_{\text{H}_2} = -2 ; \quad \nu_{\text{CH}_3\text{OH}} = +1, \quad \nu_{\text{CH}_4} = 0$$

$x = \text{fractional conversion of limiting reactant} = 0.18$

if 100% conversion is carried out

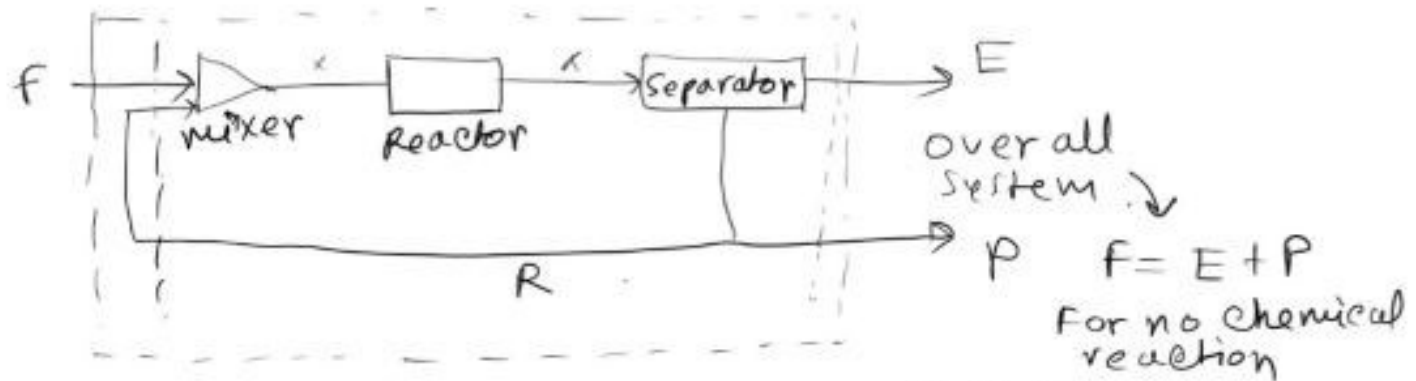
then 32.5% CO will be reacted with 65% H_2

but H_2 in the feed is 67.3% (excess).

$$= \frac{67.3 - 65}{67.3} \times 100\%$$

and CO is limiting reactant.

\therefore 18% of CO (LR) will be converted to CH_3OH .



Overall material balance for overall system

Composition balance
CO: For overall system = mixer + reactor + separator

$$F_{CO}^{out/overall} = F_{CO}^{in/overall} + \nu_{CO} \xi$$

$$[E + R + P]_{CO}^{out} = [R + F]_{CO}^{in} + \nu_{CO} \xi$$

$$\Rightarrow E \times 0 + R \cancel{y} + P y = R \cancel{y} + F \times 0.325 + (-1) \xi$$

$$\Rightarrow P y = 0.325 F - \xi \quad - (i)$$

$$\text{H}_2: E \times 0 + R \cancel{x} + P \times 0 = R \cancel{x} + F \times 0.673 + (-2) \xi$$

$$\Rightarrow P \times 0 = 0.673 F - 2 \xi \quad - \textcircled{\text{ii}}$$

$$\text{CH}_3\text{OH}: E \times 1 + R \times 0 + P \times 0 = R \times 0 + F \times 0 + (+1) \xi$$

$$\Rightarrow E = \xi \quad - \textcircled{\text{iii}}$$

$$\text{CH}_4: E \times 0 + R \times 0.032 + P \times 0.032 = R \times 0.032 + F \times 0.002$$

$$\Rightarrow 0.032 P = 0.002 F \quad - \textcircled{\text{iv}}$$

Summation of compositions

$$x + y + z = 1 \quad - \textcircled{\text{v}}$$

$$F(\xi) = x \quad \begin{array}{l} \leftarrow 0.032 \\ \hline \hline \end{array}$$

$$\Rightarrow \frac{-v_{LR} \xi}{F_{\text{reactor feed}}}_{LR} = 0.18 \quad \text{--- (vi)}$$

$LR = CO$

$$\Rightarrow \frac{-(-1) \xi}{RY + 0.325F} = 0.18$$

$$\Rightarrow 0.18 RY + 0.18 \times 0.325F = \xi \quad \text{--- (vi)}$$

$N_u = F, E, R, P, X, Y, \xi$ (7).

and $N_E = 6$ (independent equations).

$$\therefore N_D = 7 - 6 = \textcircled{1}$$

take $F = 100 \text{ kmol/hr}$

from (iv) eqn. $0.032P = 0.002F$ [CH₄]
balance

$$\Rightarrow \underline{P = 6.25 \text{ kmol/hr}}$$

So, number of equation will be $= 6 - 1 = 5$

" " variables " " $= 6 - 1 = 5$

∴ solve eqns. (i), (ii), (iii), (v), (vi)

to find E, Q, R, X, Y . $f = 100 \text{ kmol/hr}$
 $P = 6.25 \text{ "}$

$$E = 31.25 \text{ kmol/hr} \quad N_D = 0$$

$$R = 705.55 \quad "$$

$$Q = 31.25 \quad "$$

$$X = 0.768 \text{ (mole fraction) ; } H_2$$

$$Y = 0.2 \quad " ; CO$$

$$Z = 0.032 ; CH_4$$

$$X + Y + Z = 0.768 + 0.2 + 0.032 = 1 \text{ (checked)}$$

$\frac{R}{P} = C$ will be provided

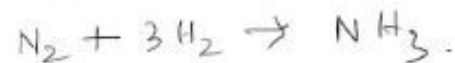
or 99% R and 1% P

or 90% R and 10% P $\frac{R}{P} = \frac{9}{1} \Rightarrow$

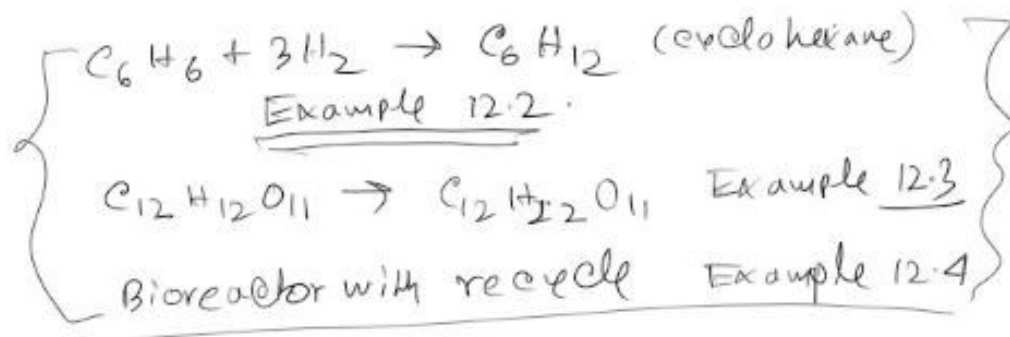
$$\therefore R = \underline{9 \times P} = 6.25 \times 9$$

here $\frac{R}{P} = \frac{705.55}{6.25}$ fixed

Various reactions can be there -



F = N_2 ; H_2 ; Ar (inert).



Elemental material balance

↳ It is different from molar or component balance



∴ molar components are $\text{CO}, \text{O}_2, \text{CO}_2$ (associated with volume change or molar change).
Elements are C, O .

↳ $F_{\text{CO}}^{\text{out}} \neq F_{\text{CO}}^{\text{in}}$ (molar balance) ↗

$F_{\text{O}_2}^{\text{out}} \neq F_{\text{O}_2}^{\text{in}}$ ||

$F_{\text{CO}_2}^{\text{out}} \neq F_{\text{CO}_2}^{\text{in}}$ ||

But for elemental balance no volume change or atomic mass change).

Each element is conserved in a reaction.

$\text{C: } F_{\text{C}}^{\text{out}} = F_{\text{C}}^{\text{in}}$ [atomic mass balance].

$\text{O: } F_{\text{O}}^{\text{out}} = F_{\text{O}}^{\text{in}}$ ||

↳ It is based on atomic mass balance of an element in a reaction (other process)

Combustion of coal in a furnace

coal compositions given from coal analysis.

Component (element)	Percent (wt.)	
C	83.05	} coal without ash = 92.64%
H	4.45	
O	3.36	
N	1.08	
S	0.70	
Ash	7.36	} Ash = 7.36%
<hr/>		Total = 100%

Take a basis of 100 lb of coal.

Orsat analysis of gas from the furnace stack is given for 24 hr time.

Component	Percent (mol %)
$\text{CO}_2 + \text{SO}_2$	15.4
CO	0
O_2	4.0
N_2	80.6

Moisture in the fuel was 3.9% (given).
(H₂O).

So, 100 lb of coal contains 3.9 lb of H₂O.

Air for burning of coal supplied which contains 0.0048 lb H₂O / lb dry air.

dry air contains N₂: 0.79 (mole fraction)
O₂: 0.21 "

$$\begin{aligned} \text{H}_2\text{O in coal} &= 3.9 \text{ lb H}_2\text{O} \\ &= 3.9 \text{ lb H}_2\text{O} \left| \frac{1 \text{ lb-mol H}_2\text{O}}{18 \text{ lb H}_2\text{O}} \right| \frac{2 \text{ lb-mol H}}{1 \text{ lb-mol of H}_2\text{O}} \\ &= \underline{0.433 \text{ lb-mol H (element)}}. \end{aligned}$$

$\frac{\text{H}_2\text{O}}{\text{H element}} = \frac{1 \text{ lb-mol}}{2 \text{ lb-mol}}$

[1 lb-mol mo H₂O contains 2 lb-mol of H }
and 1 lb-mol of O }

$$\begin{aligned} &= \frac{3.9}{18} \times 1 \text{ lb-mol O} \\ &= \underline{\underline{0.217 \text{ lb-mol O}}} \end{aligned}$$

H₂O in air:

$$= \frac{0.0048 \text{ lb H}_2\text{O}}{\text{lb of air}}$$

$$= \frac{0.0048 \text{ lb H}_2\text{O}}{\text{lb of air}} \left| \frac{29 \text{ lb of air}}{1 \text{ lb mol air}} \right| \frac{1 \text{ lb mol H}_2\text{O}}{18 \text{ lb of H}_2\text{O}}$$

29 lb = average molecular weight of air.

$$= 0.79 \times M.W_{N_2} + 0.21 \times M.W_{O_2}$$

$$= 0.79 \times 28 + 0.21 \times 32$$

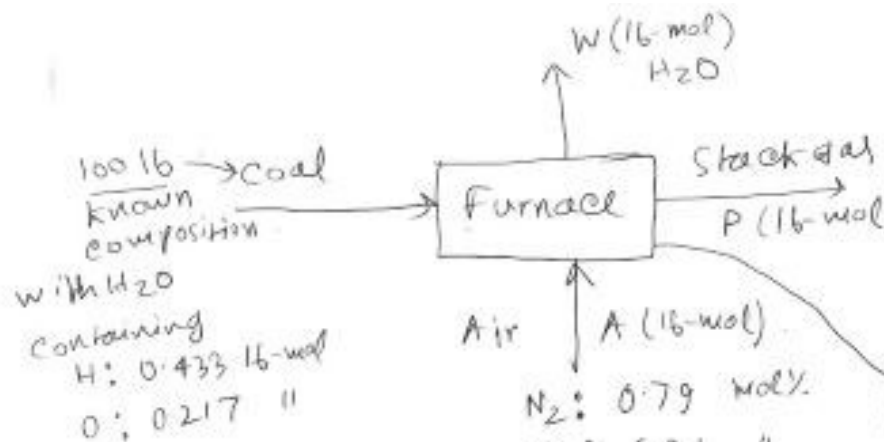
$$= 29$$

$$\text{H}_2\text{O in air} = 0.0077 \frac{\text{lb-mol H}_2\text{O}}{\text{lb mol air}}$$

$$= 2 \times 0.0077$$

$$= 0.0154 \text{ lb-mol H} / \text{lb mol air.}$$

$$= 0.0077 \text{ lb-mol O} / \text{lb-mol air.}$$



100 lb → Coal
 known composition
 with H₂O
 containing
 H: 0.433 lb-mol
 O: 0.217 "

Air A (16-mol)
 N₂: 0.79 mol%
 O₂: 0.21 "
 contaminated
 H₂O: 0.0098 lb/16 of air
 containing, H: 0.0154 lb mol/16 mol air
 O: 0.0077 "

Orsat analysis

CO ₂ + SO ₂	15.4% (mol)
CO	0%
O ₂	4%
N ₂	80.6%

Total O:
 $(0.0154 \times 2 + 0.004 \times 2) P$

Refuse R (16) { residue
 contains higher % of ash.
 S + C + H + O + N = 14%
 Ash = 86%
 14% contains (unburned same composition coal) as in coal without ash.

Ash balance

$$\frac{7.36}{\text{Feed}} = \frac{R \times 0.86}{\text{Refuse}}$$

$$R = \underline{\underline{8.56 \text{ lb}}}$$

$$\text{Unburned coal in refuse} = 8.56 \times 0.14$$

$$= \underline{1.216}$$

1.216 coal containing in the refuse
will have same composition as pure coal

pure coal

	wt%	wt fraction	lb mol		lb mol
C	83.5%	83.5/92.64	0.8964	C-	0.089648
H	4.45%	4.45/92.64	0.048	H-	0.057185
O	3.36%	3.36/92.64	0.036	O-	0.00272
N	1.02%	1.02/92.64	0.0116	N-	0.000999
S	0.7	0.7/92.64	0.00756	S-	0.000283
	<u>92.64%</u>				

$\frac{32}{16} \text{ mol} \Rightarrow$ in 1.216 coal
in R.

make elemental balances in lb-mol

$$\text{overall } F + A = W + P + R$$

feed
Air
water
Product
Residue

don't do overall but

$$C+S: \quad \cancel{F} + \cancel{A} = \cancel{W} + \cancel{P} + \cancel{R}$$

unknown
unknown
unknown

$$\begin{array}{l} H : \quad \cdot \quad \cdot \quad \cdot \quad \cdot \\ O : \quad \cdot \quad \cdot \quad \cdot \quad \cdot \\ N : \quad \cdot \quad \cdot \quad \cdot \quad \cdot \end{array}$$

$$C+S: \quad \frac{83.05}{12} + \frac{0.7}{32} + 0 = 0 + 0.154 \times P + 0.0897 + 0.0003$$

$$P = 44.54 \text{ lb-mol}$$

$$\left\{ \begin{array}{l} H : \quad \frac{4.45}{1.008} + 0.433 + 0.0154A = 2W + 0 + 0.057 \end{array} \right.$$

Coal moisture H
moisture of air
Water
 $\therefore P$
Residue

$$\begin{array}{ccccccc}
 & & A = & & & & \\
 & & \text{Coal moisture} & \text{air} & \text{air moisture} & \text{Water} & \text{F (Orsat analysis)} \\
 \text{O:} & \frac{3.36}{16} & + 0.217 & + 0.21 \times 2 \times A & + 0.007A & = W & + 2P(0.015A + 0.04) \\
 & & & & & & + 0.0027
 \end{array}$$

→ solve
H & O

$$A = 45.4 \text{ lb-mol}$$

$$W = 2.747 \text{ lb-mol}$$

$$\approx 2.75 \text{ lb-mol}$$

$$\begin{array}{ccccccc}
 & & \text{Air} & & W & \text{P, Orsat analysis} & \text{Residue, R} \\
 \text{N:} & \frac{1.08}{14} & + 2 \times 0.79A & = & 0 & + P \times 0.806 \times 2 & + 0.001 \times 2
 \end{array}$$

$$\Rightarrow \underline{19.8} = \underline{20.3} \text{ (mostly satisfied)}$$

1% error due to rounding off

$$\% \text{ excess air} = 100 \times \frac{O_2 \text{ entering} - O_2 \text{ Required}}{O_2 \text{ require}}$$

Reaction:

			lb	lbmol	Required O_2
C:	$C + O_2 \rightarrow CO_2$	CO_2	83.05	6.92	6.92
H:	$H_2 + \frac{1}{2}O_2 \rightarrow H_2O$	H_2O	4.45	4.415	1.104
	$1H \rightarrow \frac{1}{4}O$				
S:	$S + O_2 \rightarrow SO_2$	SO_2	0.7	0.022	0.022
				<hr/>	
				Total $O_2 = 8.047$ lbmol	

$$\begin{aligned} \text{O. in coal} &= \frac{3.36}{16} \text{ mol} \\ &= 0.2116 \text{ mol O.} \end{aligned}$$

$$\begin{aligned} \therefore \text{O}_2 \text{ in coal} &= \frac{0.2116}{2} \text{ mol O}_2 \\ &= 0.1058 \end{aligned}$$

$$\begin{aligned} \text{Required O}_2 &= 8.047 - \text{O}_2 \text{ in coal} \\ &= 7.9416 \text{ mol} \end{aligned}$$

$$\begin{aligned} \text{O}_2 \text{ in air} &= 45.35 \times 0.21 \\ &= 9.5235 \text{ mol} \end{aligned}$$

$$\% \text{ excess O}_2 = 100 \times \frac{9.5235 - 7.9416}{7.9416}$$

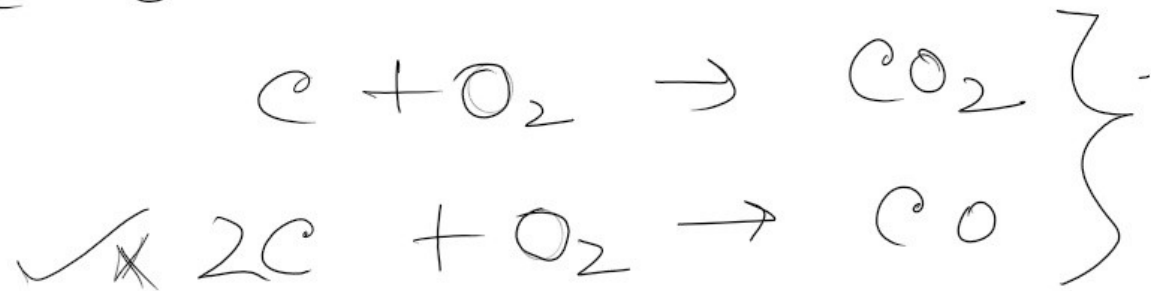
$$= \underline{\underline{19.9\%}}$$

Example 1:

Pure carbon is burned in O_2
The flue gas analysis is:

CO_2 : 75% assume it
x CO : 14% mol %
 O_2 : 11%

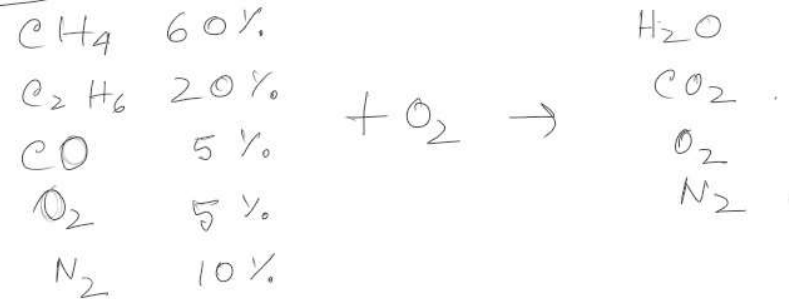
calculate % excess O_2 .



Class problem**Assignment**

A gas of following compositions
burned with 50% excess air.
calculate compositions of flue gas /
product gas.

Feed gas



Assume 100% conversions methane, ethane, and carbon monoxide.

References

- Himmelblau, D.M., Riggs, J.B., Basic Principles and Calculation in chemical engineering, Prentice Hall.