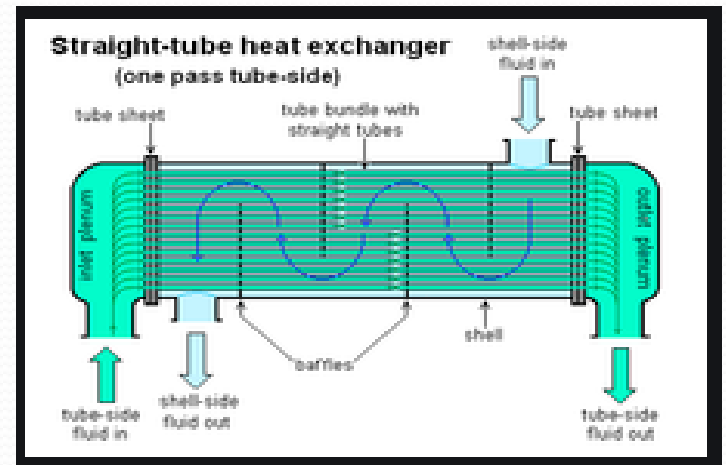
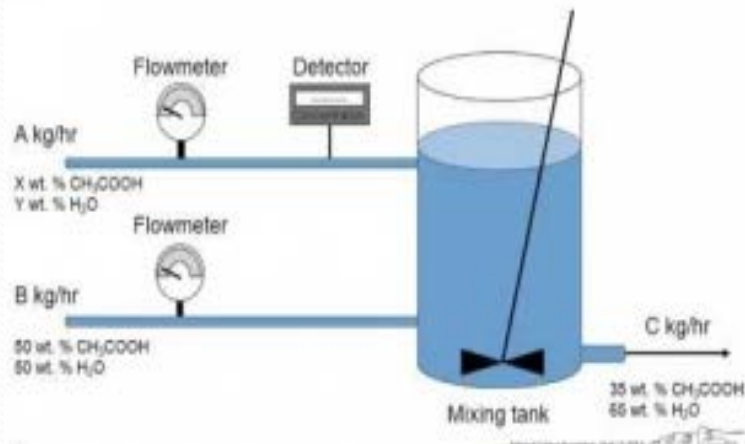
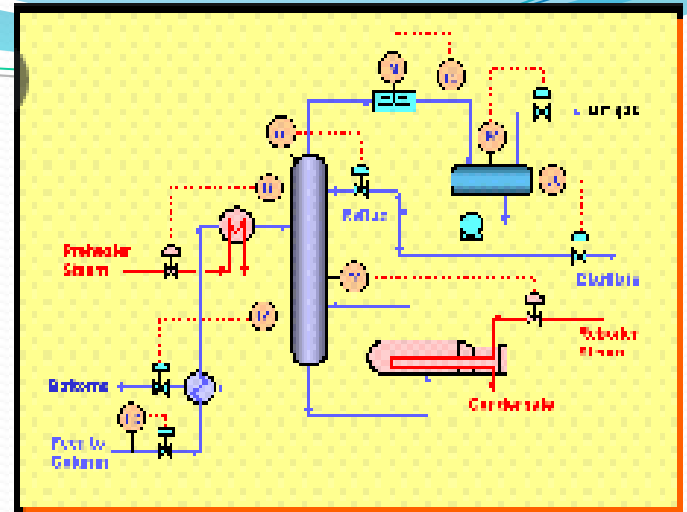
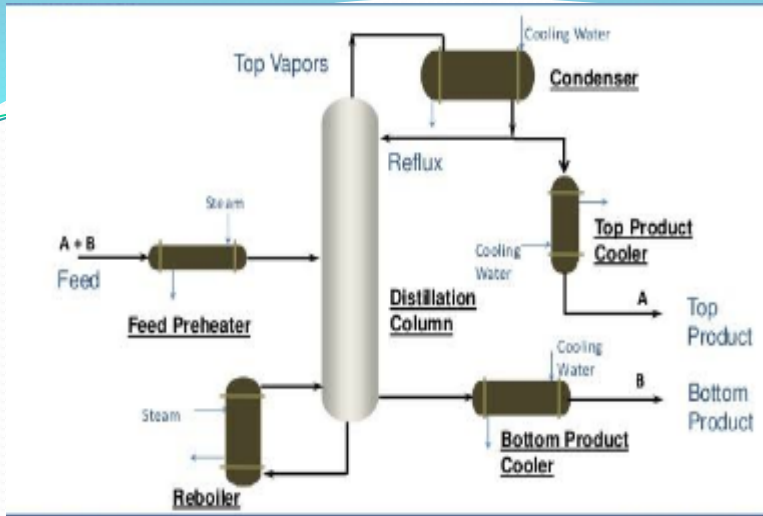


**Higher Technological Institute
Chemical Engineering Department**



Chapter 4

Material and Heat Balance



Material Balance

Material Balance Without Chemical Reaction

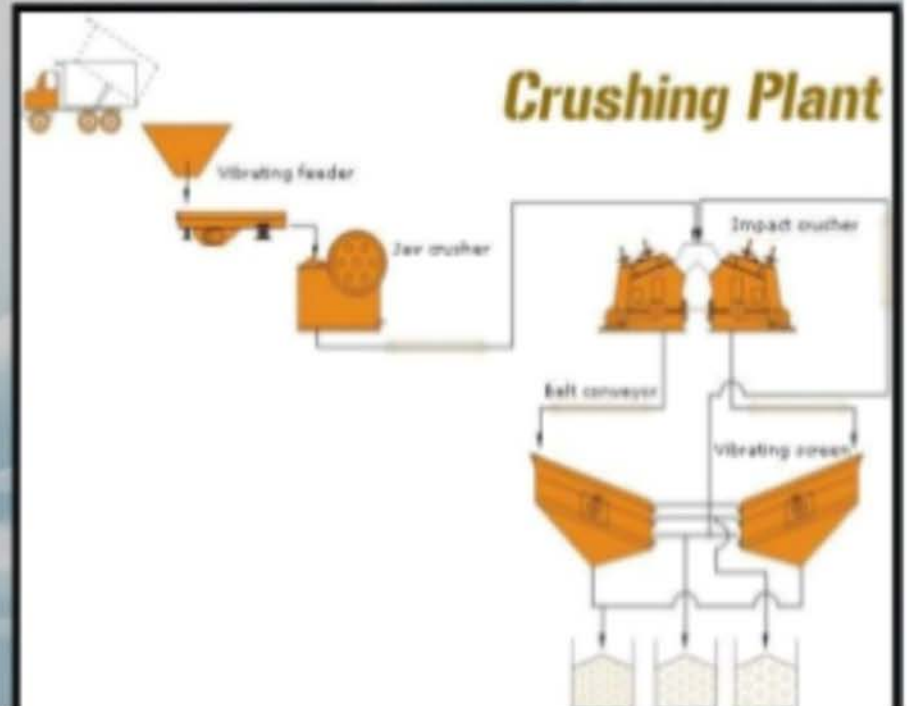
For steady state conditions

$$\sum mass\ in = \sum mass\ out$$

$$\sum moles\ in = \sum moles\ out$$

Process

- A series of actions or steps taken in order to achieve a particular end.

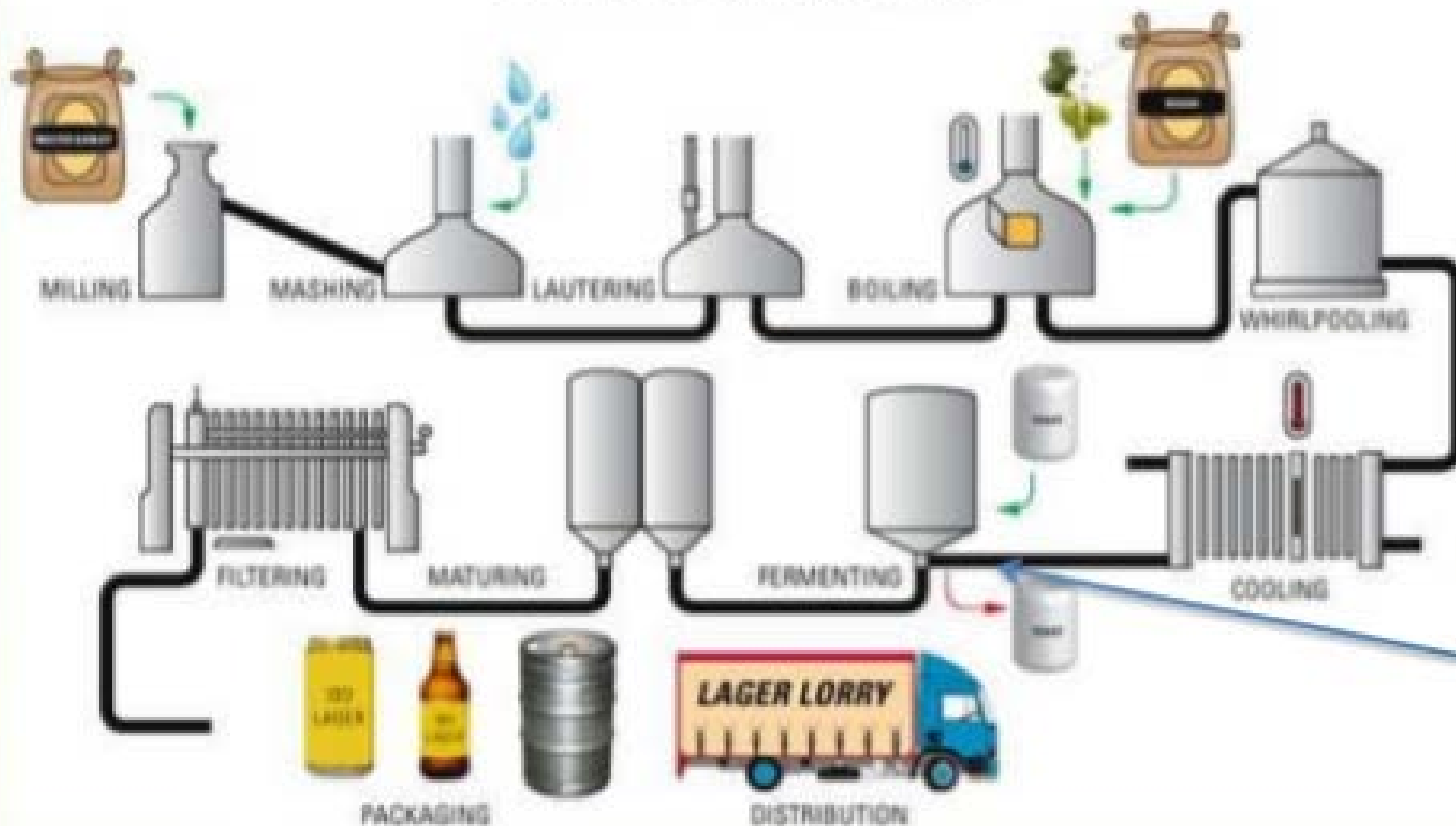


Chemical Process

...**chemical process** is a method or means of somehow changing one or more chemicals or chemical compounds. It can occur by itself or be caused by an outside force, and involves a chemical reaction of some sort...

Chemical Process Example

THE BREWERY PROCESS



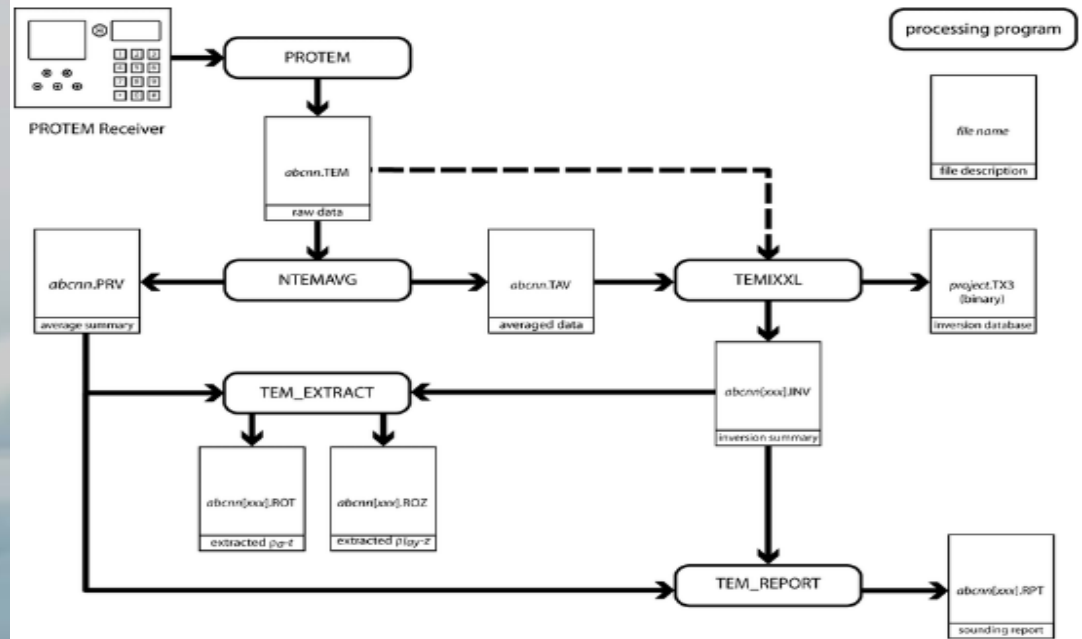
Chemical Reaction!

Block Diagram

- Simple diagram that “shows at a glance” the process
- Most used for MB solving

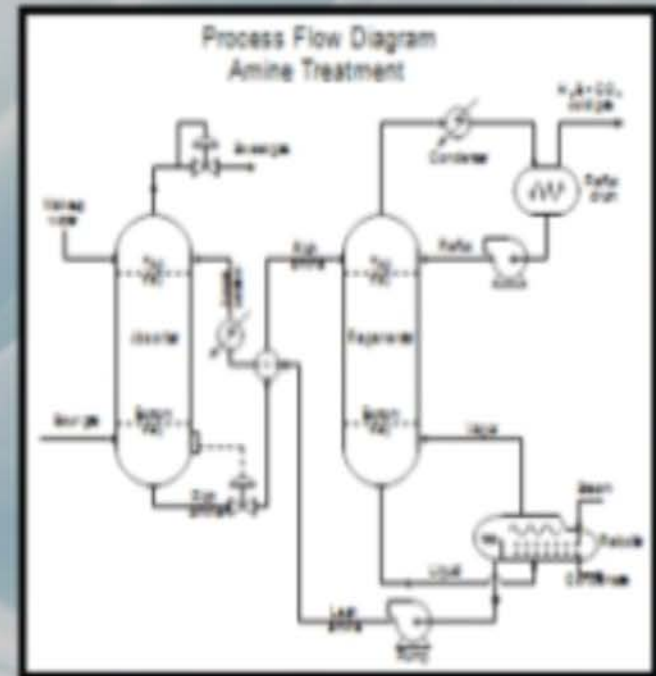
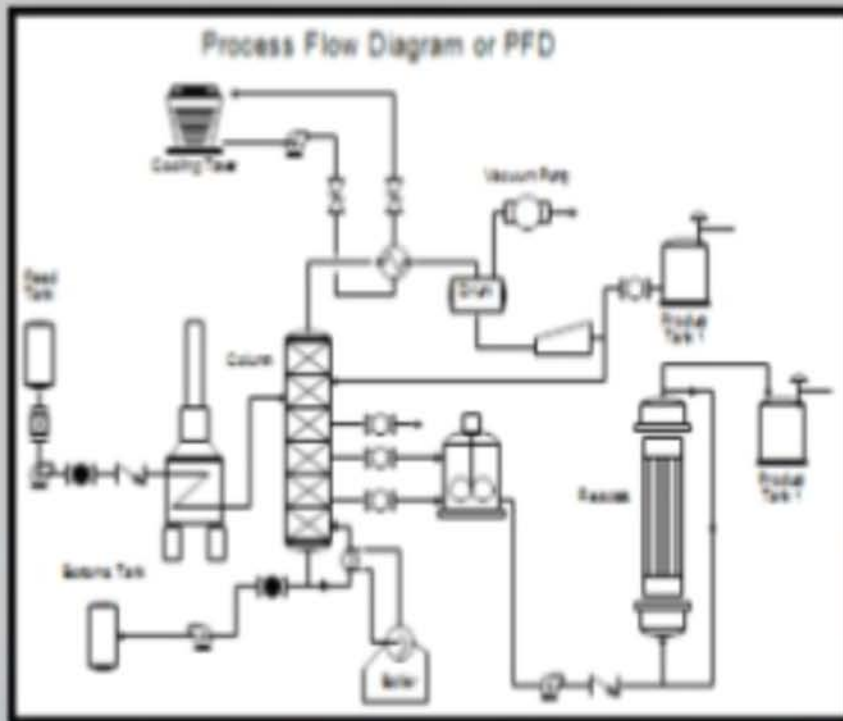
Show:

- Flows
- Unit Operations
- Some extra data



Flow Diagram

- Recommended for “general” information



- Basic Process Step in chemical engineering
- Unit operations involve:
 - physical change or chemical transformation
- Examples:
 - separation, crystallization, evaporation, filtration, polymerization, isomerization, and other reactions

Main Chemical Equipment Reactor

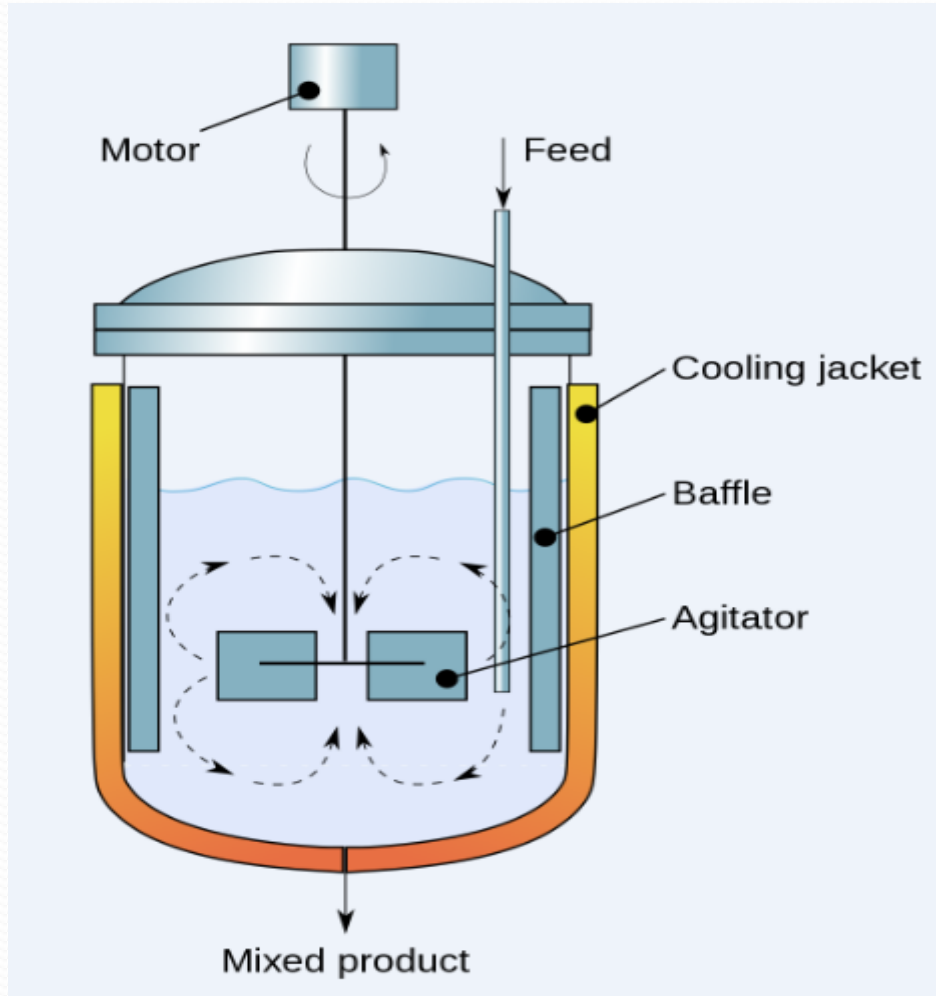


Diagram picture



Real-life picture

Distillation

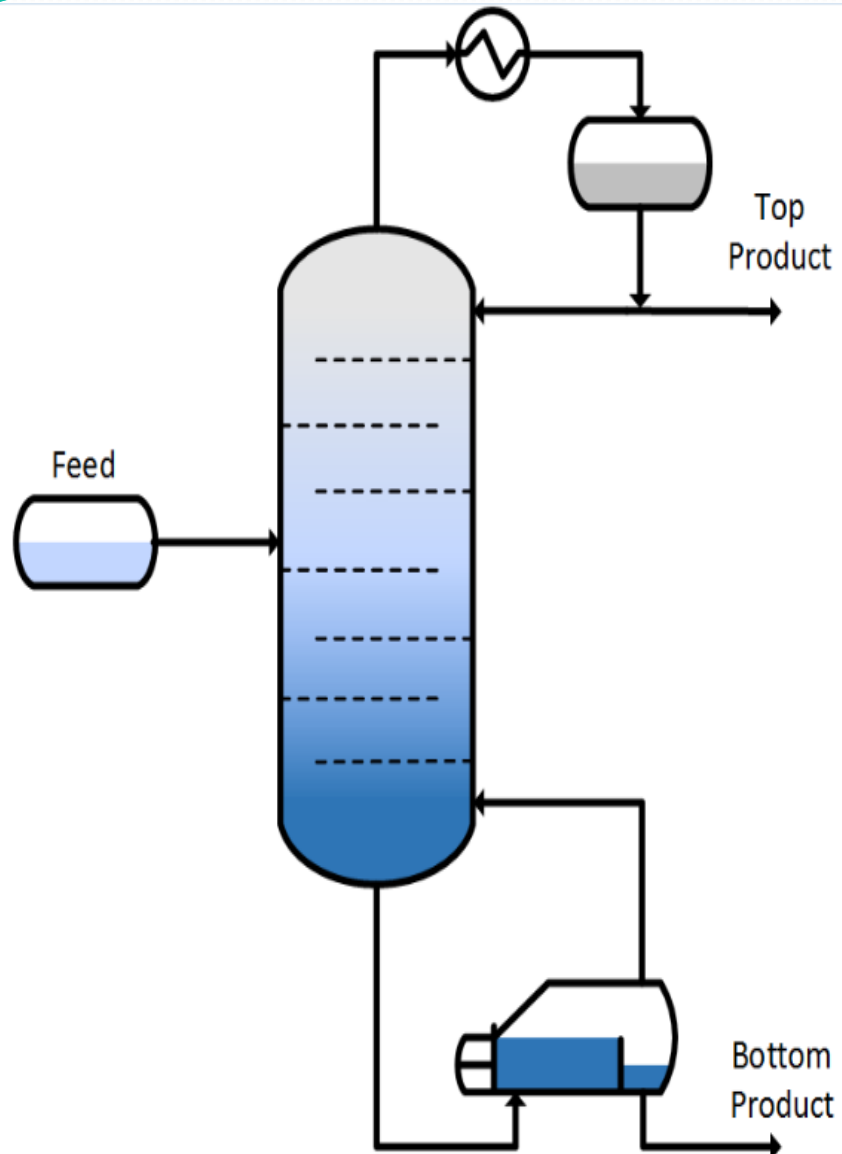


Diagram picture



Real-life picture

Unit Operations

Heat Exchanger

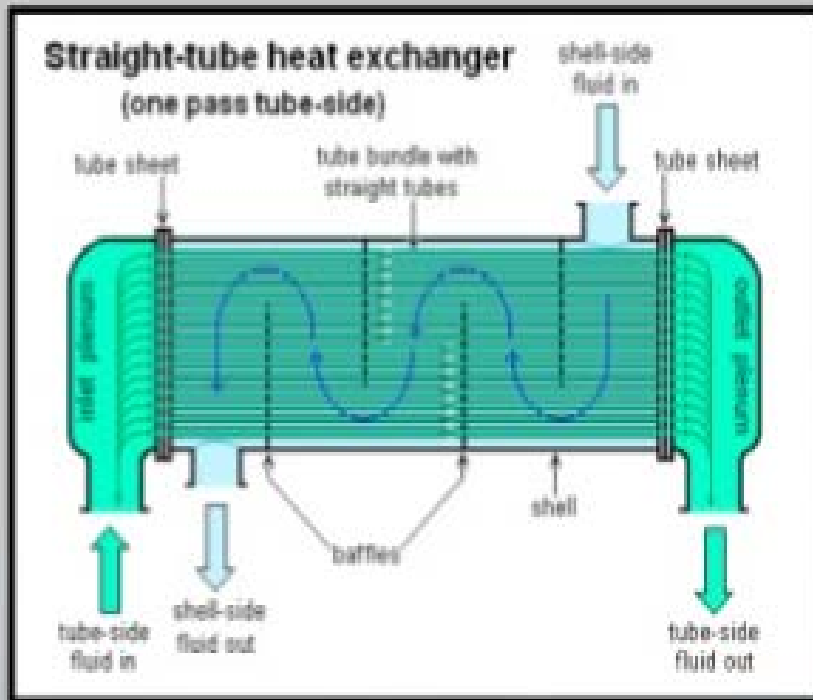


Diagram Picture



Real-Life Picture

Unit Operations

MIXER

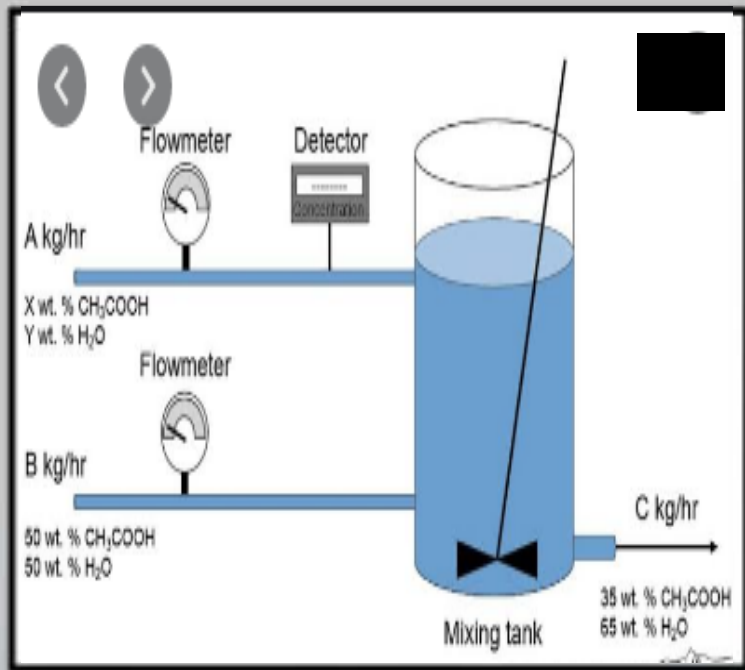


Diagram Picture



Real-Life Picture

Flow (mass, mole, volume)

- Mass flow [kg/s] = mass flow per unit time
- Mole flow [mol/s] = mole flow per unit time
- Volume flow [m³/s] = volume flow per unit time

- How much quantity of (mass/mole/volume) is “flowing” per unit time

Flow (mass, mole, volume)

- Mass flow examples:
 - 10 kg/min
 - 1 lb/s
 - 350 kTon/year
 - 3 mg per day
- Mole Flow examples:
 - 1 mol H₂O per min
 - 3.02 kmol/h
 - 125 lbmol/s
- Volume Flow examples:
 - 10 m³/s
 - 1 liter per minute
 - 4.5 ml/day
 - 18,000 gal/year

Material Balance without chemical reactions

overall material balance:

Total amount of matter into the vessel = total amount of matter out of vessel

component material balance:

Amount of components (i) into the vessel
= amount of comp. (i) out of vessel

Steady-state operation: Under steady-state, the values of all variables associated with the process do not change with time. That is, at any given location in the process, the values of temperature, pressure, composition, flow rates, etc. are independent of time. Even though a process may be steady state, it is important to realize that temperature, flow rates, or other variables may, and typically do, change from one location to another (e.g. from one process stream to another).

Solving Material Balance Problems for Single Units

Without Reaction

1. Mixer unit:

Example: It is required to prepare 1250 kg of a solution composed of 12 wt.% ethanol and 88 wt.% water. Two solutions are available, the first contains 5 wt.% ethanol, and the second contains 25 wt.% ethanol. How much of each solution are mixed to prepare the desired solution?

Solution:

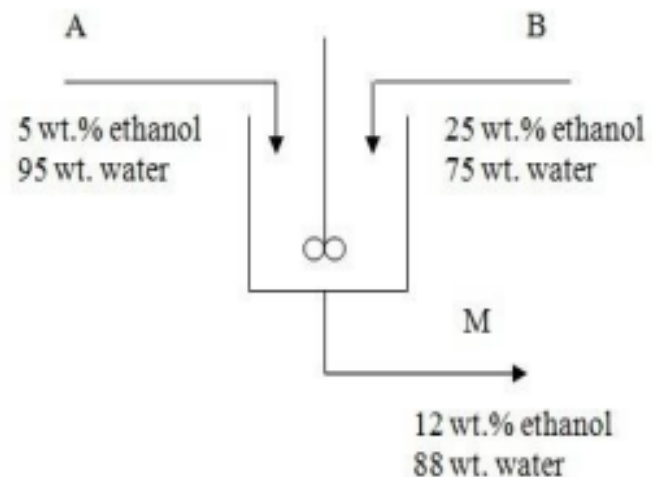
1. Ethanol balance

Input = output

$$A \left(\frac{5}{100} \right) + B \left(\frac{25}{100} \right) = M \left(\frac{12}{100} \right)$$

$$0.05 A + 0.25 B = 0.12 M$$

$$A = \left(\frac{150 - 0.25 B}{0.05} \right) = 3000 - 5 B \dots \dots \dots (1)$$



2. Water balance

Input = output

$$0.95 A + 0.75 B = 0.88 M = 0.88 (1250) = 1100$$

$$0.95 A + 0.75 B = 1100 \dots \dots \dots (2)$$

Sub. (1) in (2)

$$0.95(300 - 5 B) + 0.75 B = 1100$$

$$2850 - 4.75 B + 0.75 B = 1100$$

$$4 B = 1750 \dots \dots \dots B = \underline{437.5 \text{ kg}}$$

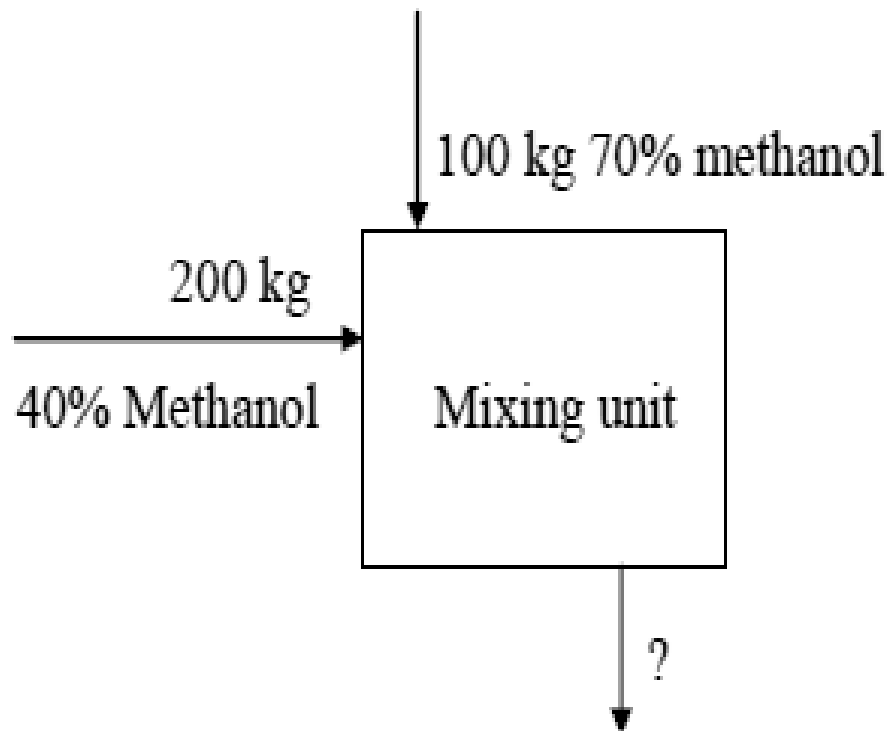
$$\text{Sub. } B \text{ in (1):} \quad A = 3000 - 5(437.5) = \underline{812.5 \text{ kg}}$$

3. Checking: Total material balance (T.M.B.), Input = $A + B = 437.5 + 812.5 = 1250 \text{ kg}$

Output = $M = 1250 \text{ kg}$

Example: Balance on a mixing unit

200 kg of a 40% w/w methanol/water solution is mixed with 100 kg of a 70% w/w methanol/water solution in a batch mixer unit. What is the final quantity and composition?



Input (Initial quantity)	=	Output (Final quantity)
---	---	--

$$\text{Total mass in} = \text{Total mass out} = 200 + 100 = 300 \text{ kg}$$

$$\text{Mass in of methanol} = \text{Mass out of methanol}$$

$$80 + 70 = \text{final methanol mass} = 150 \text{ kg}$$

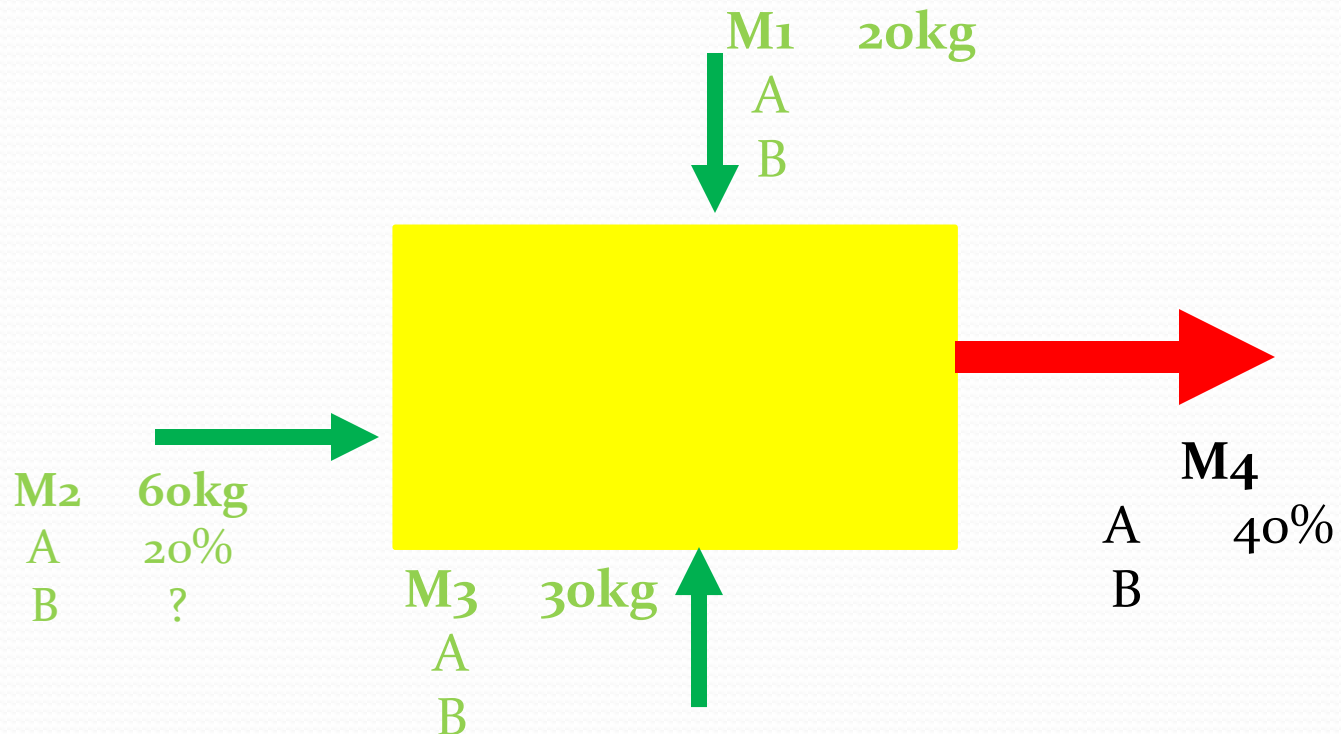
$$\text{Mass in of water} = \text{Mass out water}$$

$$120 + 30 = \text{final water mass} = 150 \text{ kg}$$

Therefore final composition of methanol is $(150/300) \times 100 = 50\%$ by wt.

Example (2): Material balances on a Mixing unit

A mixing unit is fed with three streams; the first stream is 20 Kg of mixture A and B. The second stream is 60Kg of A, B (20%A) and the third stream is 30 Kg of A and B (50%A). If the final product contains 40%A. find the composition of each stream.



Over all mass balance

$$M_1 + M_2 + M_3 = M_4$$

$$60 + 20 + 30 = M_4$$

$$M_4 = 110$$

Component Material Balance on component A

$$20 * \%A + 60 * 0.2 + 30 * 0.5 = 110 * 0.4$$

$$\%A_{M_1} = 85 \%$$

Component Material Balance on component B

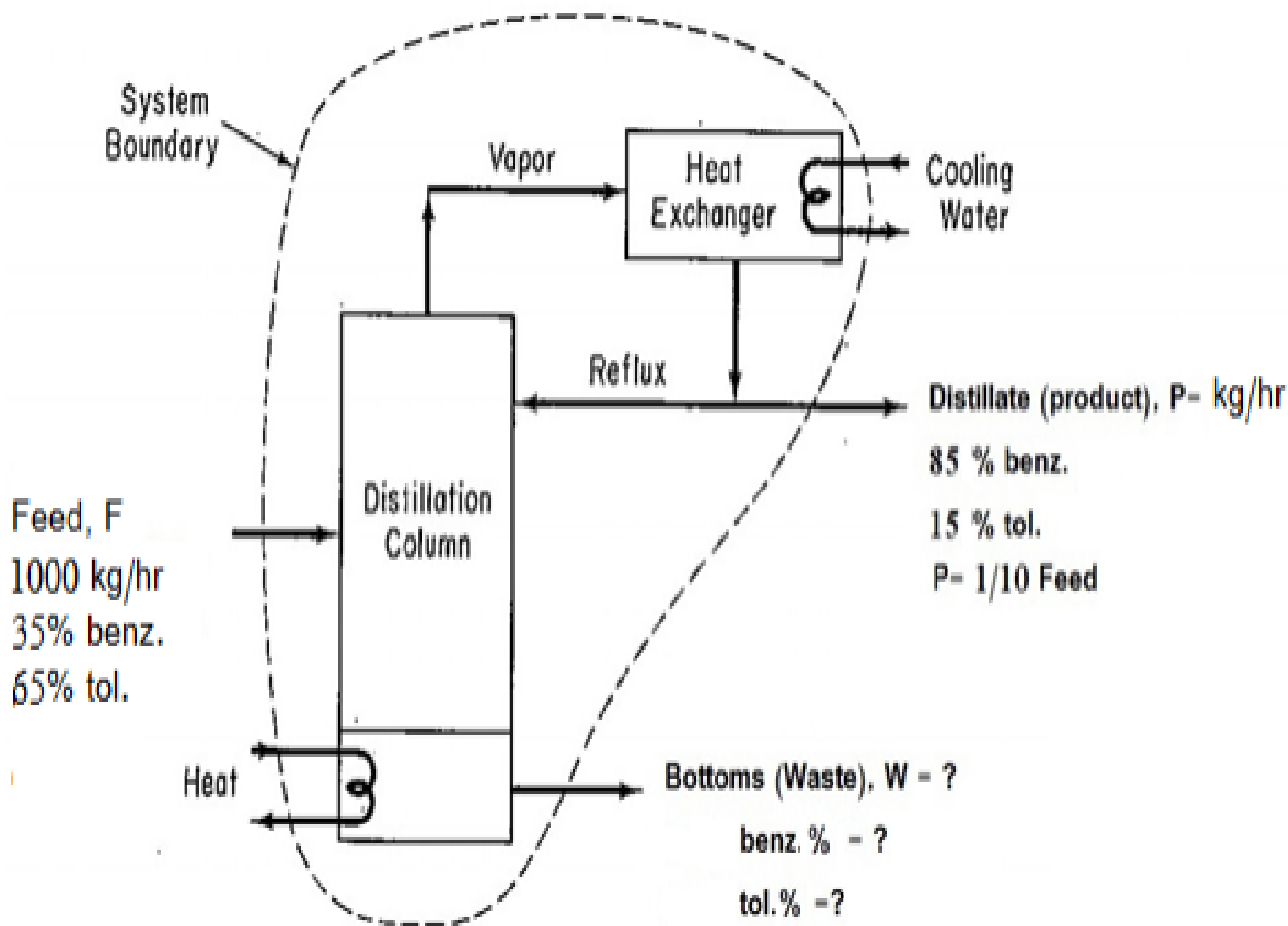
$$20 * \%B + 60 * 0.8 + 30 * 0.5 = 110 * 0.6$$

$$\%B_{M_1} = 15 \%$$

Distillation column:

Example : Overall Analysis for a Continuous Distillation Column:

A binary mixture consists of 35 % benzene and 65 % toluene are continuously fed to the distillation column at a rate of 1000 kg/hr. Whereas, the distillate flow rate was 10% from the feed flow rate. The distillate (top product) contains 85 % benzene. Calculate quantity and compositions of the waste stream.



Solution:

Although the distillation unit shown in Figure below is comprised of more than one unit of equipment, you can select a system that includes all of the equipment inside the system boundary. Consequently, you can ignore all the internal streams for this problem.

Basis: 1 hr

$$F = 1000 \text{ kg}$$

$$P = (10 / 100) \text{ of Feed} = 0.1 \times (1000) = 100 \text{ kg}$$

Overall Material Balance:

Input = Output

$$F = P + W \quad \longrightarrow \quad 1000 = 100 + W \quad \longrightarrow \quad W = 900 \text{ kg}$$

Benzene Material Balance:

$$(0.35)(1000) = (0.85)(100) + \text{Kg of benz. in (W)}$$

$$350 = 85 + \text{Kg of benz. in (W)} \quad \Longrightarrow \quad \text{Kg of benz. in (W)} = 265 \text{ kg}$$

Toluene Material Balance:

$$(0.65)(1000) = (0.15)(100) + \text{Kg of tol. in (W)}$$

$$650 = 15 + \text{Kg of benz. in (W)} \quad \Longrightarrow \quad \text{Kg of tol. in (W)} = 635 \text{ kg}$$

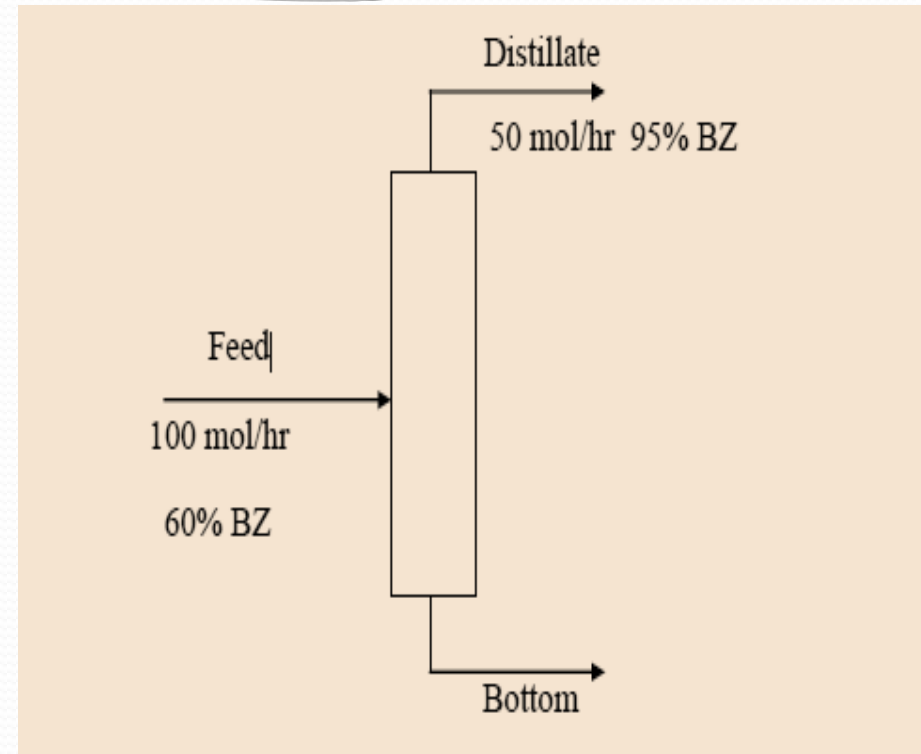
$$W = \text{Kg of benz. in (W)} + \text{Kg of tol. in (W)} = 265 + 635 = 900 \text{ kg}$$

$$\text{Mass fraction of benz. in waste} = \frac{265}{265+635} = 0.294$$

$$\text{Mass fraction of tol. in waste} = \frac{635}{265+635} = 0.706$$

Example (2): Material balances on a distillation column

A mixture of Benzene and Toluene is separated into two fractions, calculate the amount of the bottom stream and its composition.



Over all material balance

Total moles in = Total moles out

$$F = D + B$$

$$B = F - D$$

$$B = 100 - 50 = 50 \text{ mol/hr}$$

Component Material Balance

Benzene Material Balance

Moles in of benzene = Moles out of benzene

$$100 * (60/100) = 50 * (95/100) + \text{moles of benzene in bottom stream}$$

moles of benzene in bottom stream = $60 - 47.5 = 12.5 \text{ mol/hr}$

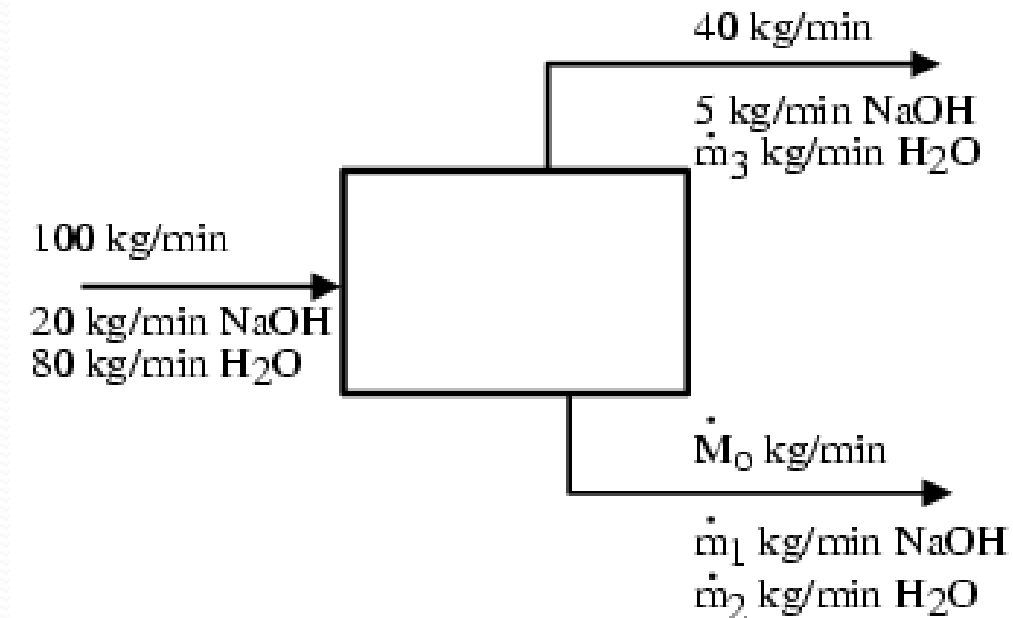
Toluene Material Balance

Moles in of toluene = Moles out of toluene

$$100 * (40/100) = 50 * (5/100) + \text{moles of toluene in bottom stream}$$

$$40 - 2.5 = 37.5 \text{ mol/hr}$$

Example (3): Material balances on a distillation column



O.M.B

$$F = D + B$$

$$100 = 40 + B$$

$$B = 60 \text{ Kg/min}$$

C.M.B on NaOH

$$20 = 5 + \text{NaOH } m^o$$

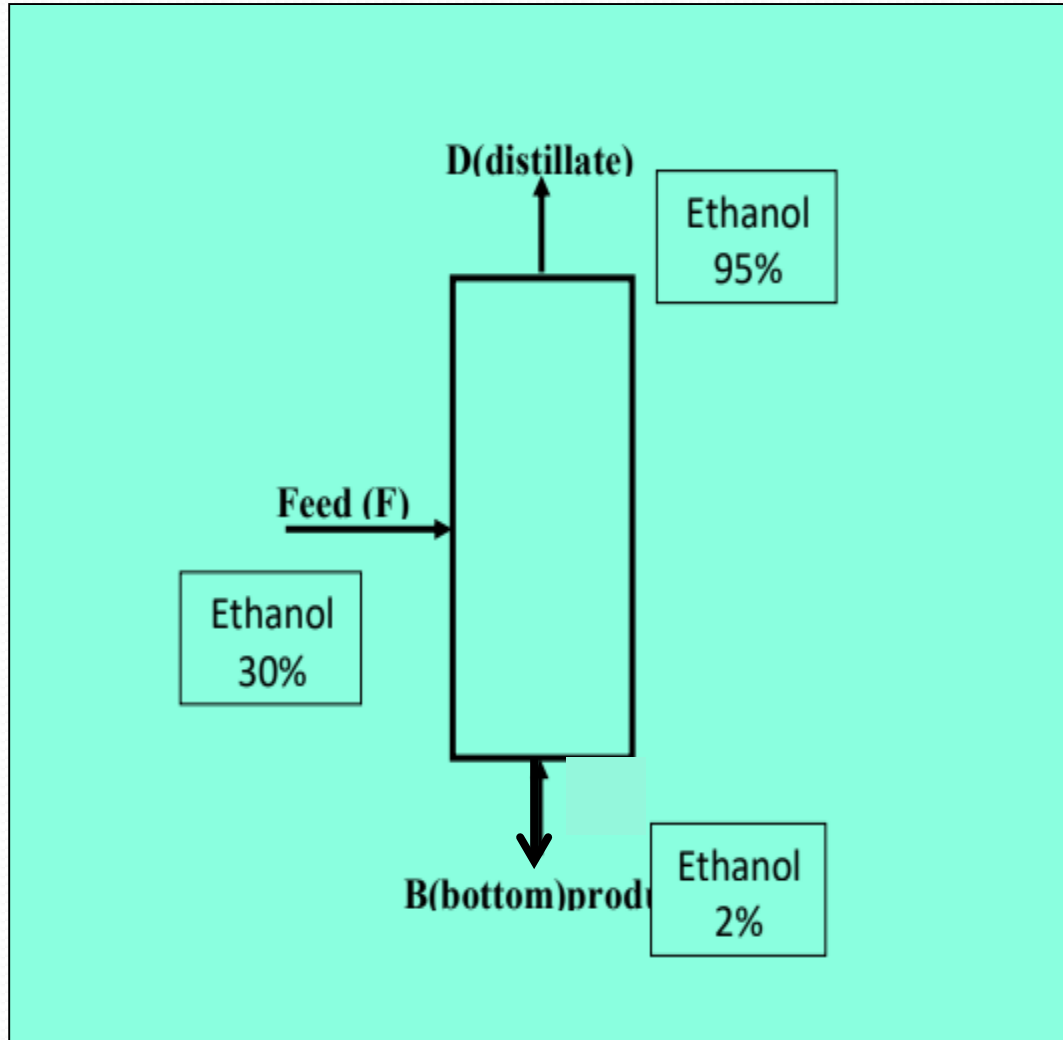
$$\text{NaOH}_B = 15 \text{ Kg/min}$$

C.M.B on H₂O

$$80 = 35 + \text{H}_2\text{O } B$$

$$\text{H}_2\text{O } B = 45 \text{ Kg/min}$$

Example (4): Material balances on a distillation column



A distillation unit is fed with 30 Kg/s with a feed containing 30% ethanol . If the concentration of ethanol in the distillate is 95 % and in bottom product is 2%, Calculate the total amount (mass) of distillate & bottom product.

Over all mass balance

$$F = D + B$$

$$30 = D + B$$

$$B = 30 - D$$

Component mass balance w.r.t ethanol

$$F * (x_{\text{ethanol}})_F = D * (x_{\text{ethanol}})_D + B * (x_{\text{ethanol}})_D$$

$$30 * 0.3 = D * 0.95 + B * 0.02$$

$$9 = 0.95 D + 0.02 B$$

$$9 = 0.95 D + 0.02(30 - D)$$

$$9 = 0.95 D + 0.6 + 0.02 D$$

$$8.4 = 0.93 D$$

$$B = 30 - 9.03$$

$$D = 9.03 \text{ Kg}$$

$$B = 20.97 \text{ Kg}$$

Material Balance for Reacting system

The Chemical Reaction Equation and Stoichiometry

$$\sum \text{mass in} = \sum \text{mass out}$$

$$\sum \text{moles in} \neq \sum \text{moles out}$$



MB in Combustion

- **Combustion:** is a high-temperature exothermic chemical reaction between a fuel and an oxidant, usually atmospheric oxygen, that produces oxidized, often gaseous products
- Why burning? To get heat energy → electrical energy → electricity!

MB in Combustion

Reactants:

- Fuel
- Oxygen
- Inerts (don't react)

Products:

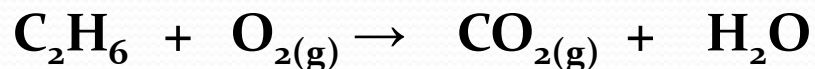
- CO_2
- H_2O
- Inerts (flow out)

- General idea:
- Fuel + Oxygen \rightarrow CO_2 + H_2O + Heat
- Ex: $\text{CH}_4 + \text{O}_2 \rightarrow \text{CO}_2 + \text{H}_2\text{O}$ (not balanced)
- Tips for balancing (order)
 - Balance all Carbon atoms
 - Balance all Hydrogen Atoms
 - Balance all Oxygen Atoms (don't hesitate to use fractions in moles)

MB in Combustion

- Example: Propane
- $C_3H_8 + O_2 \rightarrow CO_2 + H_2O$
 - Balance C: $C_3H_8 + O_2 \rightarrow 3CO_2 + H_2O$
 - Balance H: $C_3H_8 + O_2 \rightarrow 3CO_2 + 4H_2O$
 - Balance O: $C_3H_8 + 5 \cdot O_2 \rightarrow 3CO_2 + 4H_2O$

the combustion reaction for Ethane as an example



If the molar mass of C = 12, H = 1, O = 16

Balance C: $\text{C}_2\text{H}_6 + \text{O}_{2(g)} \rightarrow 2\text{CO}_{2(g)} + \text{H}_2\text{O}$
 Balance H: $\text{C}_2\text{H}_6 + \text{O}_{2(g)} \rightarrow 2\text{CO}_{2(g)} + 3\text{H}_2\text{O}$
 Balance O: $\text{C}_2\text{H}_6 + 3.5\text{O}_{2(g)} \rightarrow 2\text{CO}_{2(g)} + 3\text{H}_2\text{O}$
To get the balanced equation:



$$\text{Mass in} = 1 \times 30 + 3.5 \times 32 = 142 \text{ gm}$$

$$\text{Mass out} = 2 \times 44 + 3 \times 18 = 142 \text{ gm}$$

Molecular weight:-

$$\text{C}_2\text{H}_6 = 2 \times 12 + 6 \times 1 = 30$$

$$\text{O}_2 = 2 \times 16 = 32$$

$$\text{CO}_2 = 12 + 2 \times 16 = 44$$

$$\text{H}_2\text{O} = 2 \times 1 + 16 = 18$$

Remember

$$\sum \text{mass in} = \sum \text{mass out}$$

$$\sum \text{moles in} \neq \sum \text{moles out}$$

Remember

mole in \neq mole out

$$1+3.5 \neq 2+3$$

Concept of Excess Air

- For optimum combustion, the real amount of combustion air must be greater than that required theoretically. This additional amount of air is called “excess air”.
- A certain amount of excess air is needed for complete combustion of fuel.
- Too much excess air leads to heat losses and too little excess air leads to incomplete combustion.
- You can tell if there is too little or too much excess air by measuring the CO_2 in the flue gases.
- The amount of excess air required depend on various factors like type of fuel used, type of firing system, size of fuel in case of solid fuel etc.

% of Excess Oxygen

- Express the excess in %

$$\% \text{ Excess Oxygen} = [\text{Oxygen feed} - \text{Oxygen (theoretical)}] / [\text{Oxygen (theoretical)}]$$

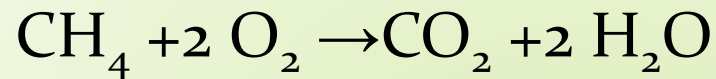
- So a 20% oxygen excess for CH₄ would be:

$$20\% = (\text{Oxygen feed} - 4 \text{ mol O}_2) / (4 \text{ mol O}_2)$$

$$0.2 \cdot 4 = \text{O} - 4$$

$$\text{O} = 4 + 0.8 = 4.8 \text{ moles of O}_2$$

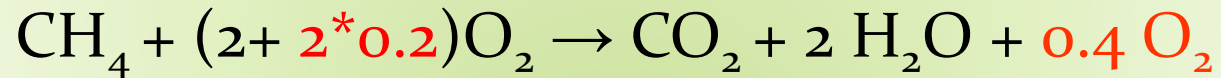
Use of excess of one component of reactants



This is the stoichiometric reaction; but usually we use excess of one of the components.

If we use 20 % excess of oxygen,

then the reaction will be



Example

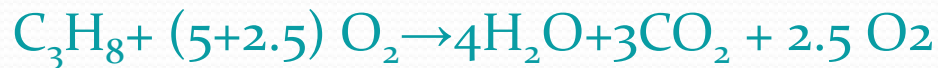
Propane (C_3H_8) burns in this reaction:



50% excess O_2

If 200 g of propane is burned, how many g of H_2O is produced?

Answer:  Actual wt.



Theoretical wt.

$$44 \cdot 1 \quad 7.5 \cdot 32 \quad 4 \cdot 18 \quad 3 \cdot 44 \quad 2.5 \cdot 32$$

Actual wt..

$$200 \quad x$$

$$\text{Actual wt. } O_2 \text{ reactant} = (200 \cdot 7.5 \cdot 32) / 44 = 1090.9 \text{ gm}$$

$$\text{Actual wt. } H_2O = (200 \cdot 4 \cdot 18) / 44 = 327.27 \text{ gm}$$

$$\text{Actual wt. } CO_2 = (200 \cdot 3 \cdot 44) / 44 = 600 \text{ gm}$$

$$\text{Actual wt. } O_2 \text{ product} = (200 \cdot 2.5 \cdot 32) / 44 = 363.63 \text{ gm}$$

Energy Balance

Physical Process (Without Chemical Reaction)

i. Without any phase change

The energy lost or gained is given by:

$$E = \int_{T_1}^{T_2} m C_p dT$$

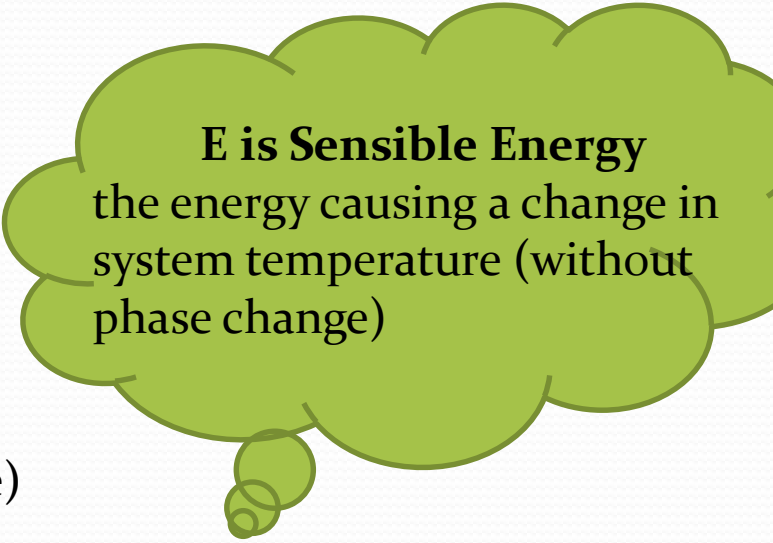
m mass or mole of the fluid (kg) or (kmole)

C_p Specific heat capacity of the fluid (kJ/kg K) or (kJ/kmol K)

If the specific heat doesn't vary with temperature

$$E = m C_p \Delta T$$

Δt temperature difference



E is Sensible Energy
the energy causing a change in
system temperature (without
phase change)

ii. With Phase Change

The energy lost or gained is given by:

Latent energy
The energy that causes
change in the phase
without change in
temperature

$$E = m C_p \Delta T + m' \times \text{latent heat}$$

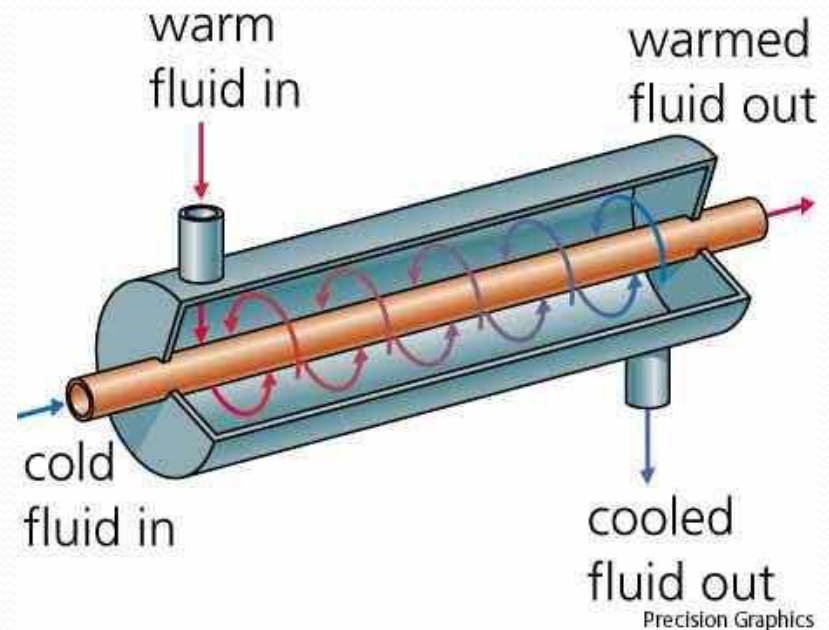
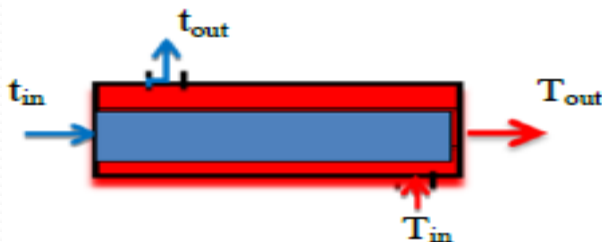
m Total mass of the fluid (kg)

m' mass of the fluid changing its phase

Heat Exchanger

The energy balance is calculated according to:

$$\text{Heat lost} = \text{Heat gained}$$



Example 1

Calculate the mass of hot oil required to raise the temperature of 200 kg water from 20 °C to 70 °C ; given that:

- C_p for water = 4.18 kJ /kg °C
- C_p for oil = 2.1
- Initial temperature of oil = 120 °C
- Final temperature of oil = 90 °C

$$\text{heat lost} = \text{heat gained}$$

and since no phase change occurs.

$$m_{\text{water}} * c_{p \text{ water}} (70 - 20) = m_{\text{oil}} * c_{p \text{ oil}} (120 - 90)$$

$$200 * 4.18 * 50 = m_{\text{oil}} * 2.1 * 30$$

$$m_{\text{oil}} = 663.5 \text{ kg.}$$

Example 2

Calculate the mass of hot oil used for heating 600 Kg of milk from 4 °C to 82 °C given that:

- $C_{p\text{milk}} = 4.3 \text{ kJ/Kg } ^\circ\text{C}$,
- $C_{p\text{oil}} = 1.8 \text{ kJ/Kg } ^\circ\text{C}$,
- Initial temperature of oil = 150 °C ,
- Final temperature of oil = 90 °C

$$m_{\text{milk}} \times C_{p\text{milk}} \times (t_{\text{out}} - t_{\text{in}}) = m_{\text{oil}} \times C_{p\text{oil}} \times (T_{\text{in}} - T_{\text{out}})$$

$$600 \times 4.3 \times (82 - 4) = m_{\text{oil}} \times 1.8 \times (150 - 90)$$

$$m_{\text{oil}} = 1863.33 \text{ Kg}$$

Example 3

Calculate the mass of component (A) with $C_p = 2.1 \text{ kJ/kg}^\circ\text{C}$, cooling by 200 kg cold water from 50°C to 25°C , the cooled water enter the heat exchanger at 4°C and out at 20°C , $C_{p\text{water}} = 4.18 \text{ kJ/kg}^\circ\text{C}$

$$m_A \times C_{p_A} \times (T_{in} - T_{out}) = m_{\text{water}} \times C_{p_{\text{water}}} \times (t_{out} - t_{in})$$

$$m_A \times 2.1 \times (50 - 25) = 200 \times 4.18 \times (20 - 4)$$

$$M_A = 254.78 \text{ Kg}$$

Energy Balance

With Chemical Reaction

The heat of reaction is produced or absorbed during chemical reactions. The value of the enthalpy change reported for a reaction is the amount of heat released or absorbed when reactants are converted to products

Enthalpies of Chemical Change

Enthalpy

- is a state function whose value depends only on the current state of the system, not on the path taken to arrive at that state
- $\Delta H = H_{\text{products}} - H_{\text{reactants}}$
- The physical states of reactants and products must be specified as solid (*s*), liquid (*l*), gaseous (*g*), or aqueous (*aq*) when enthalpy changes are reported

When the heat of reaction is measured under

Standard Thermodynamic Conditions

- 1 atm pressure
- *specified temperature usually 25 C,*
- *1 M concentration for all substance in solution*

is called a ***standard heat of reaction*** and is indicated by the symbol ΔH°_r .

We can calculate the heat of reaction using different methods

1. By the knowledge of heat of formation of both reactants and products.
2. Using Hess's law
3. By using the bond dissociation energy.

1. By the knowledge of heat of formation of both reactants and products

The Standard heat of formation Is the enthalpy change for the formation of 1 mol of a substance in its standard state from its constituent elements in their standard states.

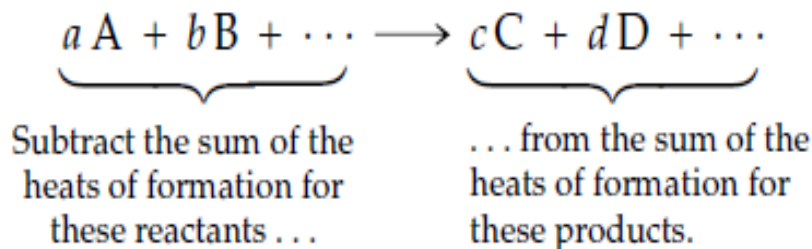


Substance	Formula	ΔH_f° (kJ/mol)	Substance	Formula	ΔH_f° (kJ/mol)
Acetylene	$\text{C}_2\text{H}_2(g)$	226.7	Hydrogen chloride	$\text{HCl}(g)$	-92.3
Ammonia	$\text{NH}_3(g)$	-46.1	Iron(III) oxide	$\text{Fe}_2\text{O}_3(s)$	-824.2
Carbon dioxide	$\text{CO}_2(g)$	-393.5	Magnesium carbonate	$\text{MgCO}_3(s)$	-1095.8
Carbon monoxide	$\text{CO}(g)$	-110.5	Methane	$\text{CH}_4(g)$	-74.8
Ethanol	$\text{C}_2\text{H}_5\text{OH}(l)$	-277.7	Nitric oxide	$\text{NO}(g)$	90.2
Ethylene	$\text{C}_2\text{H}_4(g)$	52.3	Water (g)	$\text{H}_2\text{O}(g)$	-241.8
Glucose	$\text{C}_6\text{H}_{12}\text{O}_6(s)$	-1260	Water (l)	$\text{H}_2\text{O}(l)$	-285.8

N.B. The heat of formation of element is equal zero.

$$\Delta H^{\circ}_{\text{reaction}} = \Delta H^{\circ}_{\text{f}}(\text{Products}) - \Delta H^{\circ}_{\text{f}}(\text{Reactants})$$

To find ΔH° for the reaction



$$\Delta H^{\circ}_{\text{reaction}} = [c\Delta H^{\circ}_{\text{f}}(\text{C}) + d\Delta H^{\circ}_{\text{f}}(\text{D}) + \dots] - [a\Delta H^{\circ}_{\text{f}}(\text{A}) + b\Delta H^{\circ}_{\text{f}}(\text{B})]$$

For example, let's calculate ΔH° for the fermentation of glucose to make ethyl alcohol (ethanol), the reaction that occurs during the production of alcoholic beverages:



Using the data in Table 8.2 gives the following answer:

$$\begin{aligned} \Delta H^{\circ} &= [2 \Delta H^{\circ}_{\text{f}}(\text{Ethanol}) + 2 \Delta H^{\circ}_{\text{f}}(\text{CO}_2)] - [\Delta H^{\circ}_{\text{f}}(\text{Glucose})] \\ &= (2 \text{ mol})(-277.7 \text{ kJ/mol}) + (2 \text{ mol})(-393.5 \text{ kJ/mol}) - (1 \text{ mol})(-1260 \text{ kJ/mol}) \\ &= -82 \text{ kJ} \end{aligned}$$

The fermentation reaction is exothermic by 82 kJ.

The standard heat of reaction ΔH° is calculated according to the equation.

$$\Delta H^\circ = \sum \text{heat of formation of products} \\ - \sum \text{heat of formation of reactants.}$$



$$\Delta H^\circ_r = [2 \times (H_{fC}) + 1 \times (H_{fD})] - [2 \times (H_{fA}) + 3 \times (H_{fB})]$$

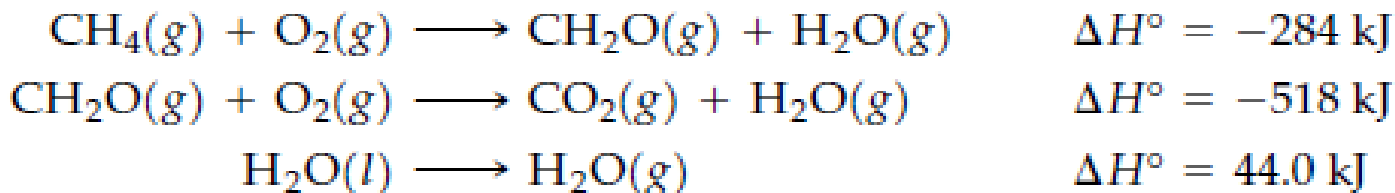
2. Using Hess's Law

HESS'S LAW The overall enthalpy change for a reaction is equal to the sum of the enthalpy changes for the individual steps in the reactions. Reactants and products in the individual steps can be added and subtracted like algebraic quantities in determining the overall equation

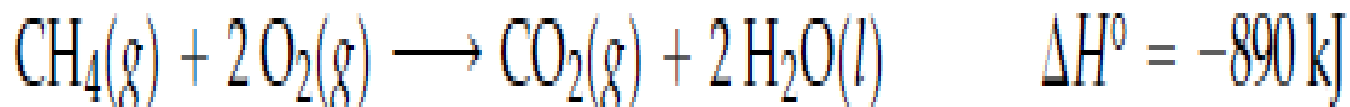
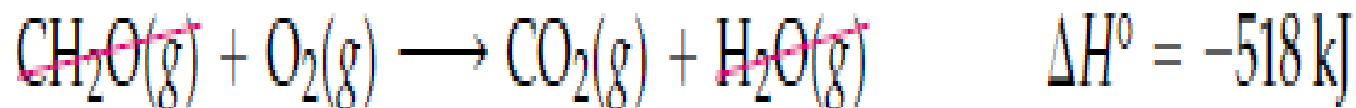
Methane, the main constituent of natural gas, burns in oxygen to yield carbon dioxide and water:



Use the following information to calculate ΔH° (in kilojoules) for the combustion of methane:



SOLUTION

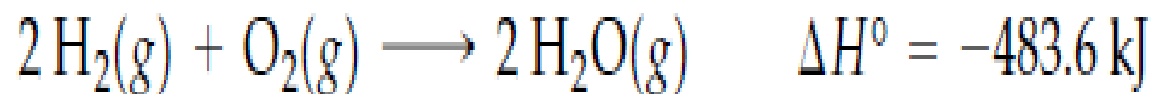


Water gas is the name for the industrially important mixture of CO and H₂ prepared by passing steam over hot charcoal at 1000°C:



“Water gas”

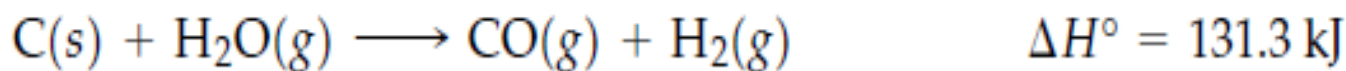
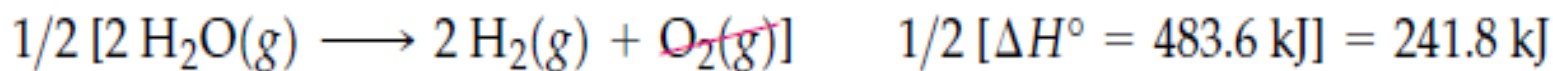
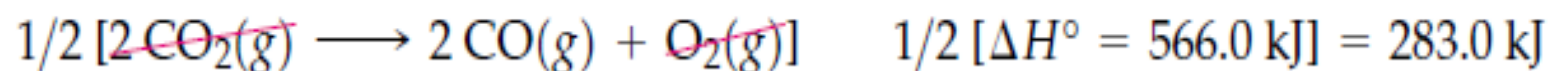
The hydrogen is then purified and used as a starting material for preparing ammonia. Use the following information to calculate ΔH° (in kilojoules) for the water-gas reaction:



STRATEGY

As in Worked Example 8.6, the idea is to find a combination of the individual reactions whose sum is the desired reaction. In this instance, it's necessary to reverse the second and third steps and to multiply both by $1/2$ to make the overall equation balance. In so doing, the sign of the enthalpy changes for those steps must be changed and also multiplied by $1/2$. (Alternatively, we could multiply the first step by 2 and then divide the final result by 2.) Note that $\text{CO}_2(\text{g})$ and $\text{O}_2(\text{g})$ cancel because they appear on both the right and left sides of reactions.

SOLUTION



The water-gas reaction is endothermic by 131.3 kJ.

3. By using the bond dissociation energy.

For the reaction $X-Y \longrightarrow X + Y$ $\Delta H^{\circ} = D = \text{Bond dissociation energy}$

Bond dissociation energies are always positive because energy must always be put into a bond to break it.

$$\Delta H^{\circ} = D(\text{Reactant bonds}) - D(\text{Product bonds})$$

ΔH is called the dissociation energy of the bond X – Y.

For a certain chemical reaction, the standard heat of reaction

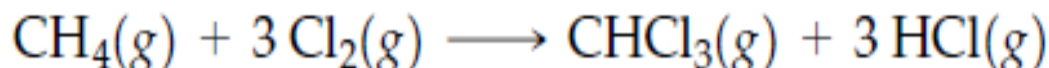
ΔH°

$$\Delta H^\circ = \Sigma D (\text{reactant bonds}) - \Sigma D (\text{product bonds})$$



$$\Delta H^\circ = [D (\text{H} - \text{H}) + D (\text{Cl} - \text{Cl})] - 2 \times D (\text{H} - \text{Cl})]$$

Use the data in Table 7.1 to find an approximate ΔH° (in kilojoules) for the industrial synthesis of chloroform by reaction of methane with Cl_2 .



STRATEGY

Identify all the bonds in the reactants and products, and look up the appropriate bond dissociation energies in Table 7.1. Then subtract the total energy of the product bonds from the total energy of the reactant bonds to find the enthalpy change for the reaction.

SOLUTION

The reactants have four C–H bonds and three Cl–Cl bonds; the products have one C–H bond, three C–Cl bonds, and three H–Cl bonds. The bond dissociation energies from Table 7.1 are:

$$\text{C—H} \quad D = 410 \text{ kJ/mol}$$

$$\text{Cl—Cl} \quad D = 243 \text{ kJ/mol}$$

$$\text{C—Cl} \quad D = 330 \text{ kJ/mol}$$

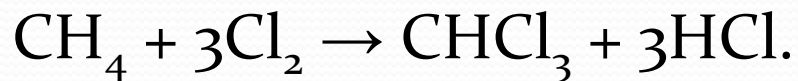
$$\text{H—Cl} \quad D = 432 \text{ kJ/mol}$$

Subtracting the total energy of the product bonds from the total energy of the reactant bonds gives the enthalpy change for the reaction:

$$\begin{aligned}\Delta H^\circ &= [3 D_{\text{Cl}-\text{Cl}} + 4 D_{\text{C}-\text{H}}] - [D_{\text{C}-\text{H}} + 3 D_{\text{H}-\text{Cl}} + 3 D_{\text{C}-\text{Cl}}] \\ &= [(3 \text{ mol})(243 \text{ kJ/mol}) + (4 \text{ mol})(410 \text{ kJ/mol})] - [(1 \text{ mol})(410 \text{ kJ/mol}) + \\ &\quad (3 \text{ mol})(432 \text{ kJ/mol}) + (3 \text{ mol})(330 \text{ kJ/mol})] \\ &= -327 \text{ kJ}\end{aligned}$$

The reaction is exothermic by approximately 330 kJ.

Calculate the standard heat of the following reaction



Given that:

C – H D = 410 KJ / mole.

C – Cl D = 330 KJ / mole.

Cl – Cl D = 243 KJ / mole.

H – Cl D = 432 KJ / mole.

Solution

$$\begin{aligned}\Delta H_r^0 &= [3 \times D (\text{Cl} - \text{Cl}) + 4 \times D (\text{C} - \text{H})] - [D (\text{C} - \text{H}) + \\ &3 \times D (\text{C} - \text{Cl}) + 3 \times D (\text{H} - \text{Cl})] \\ &= [3 \times 243 + 4 \times 410] - [1 \times 410 + 3 \times 432 + 3 \times \\ &330] = - 327 \text{ KJ}.\end{aligned}$$