B Sc SEM VI (Program): DCE
Dynamic Stereochemistry

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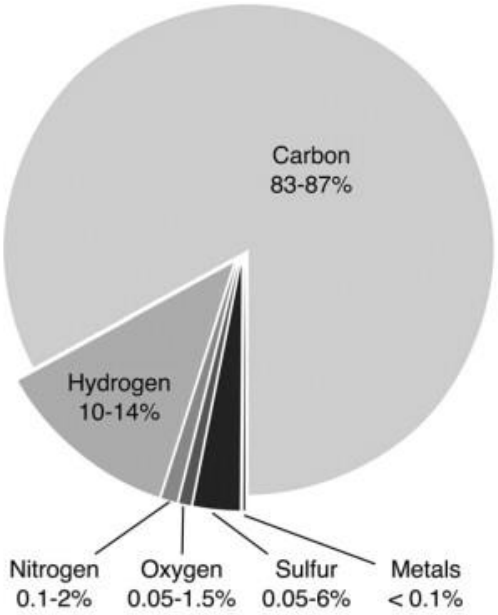
Petroleum and Petrochemical Industry (10 L)

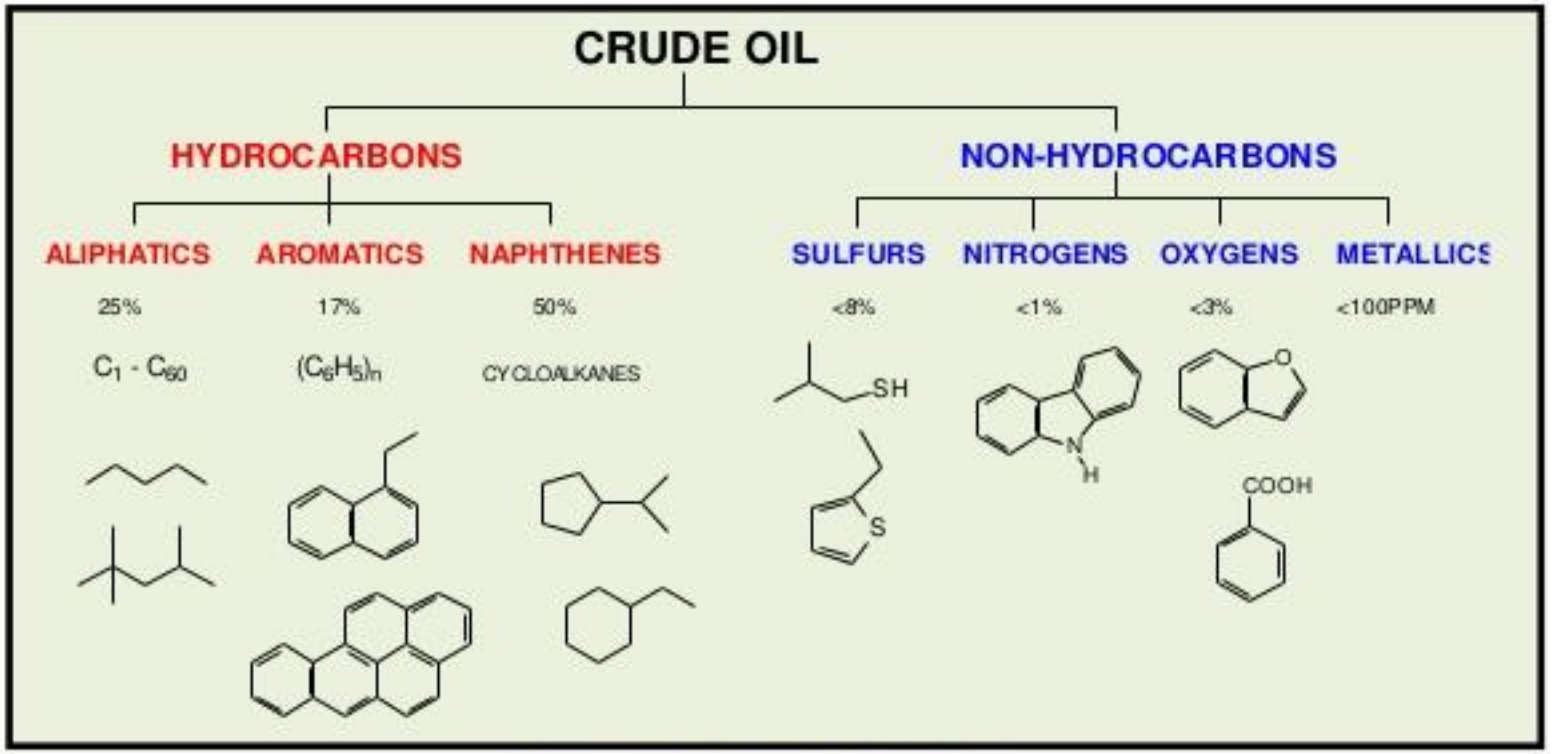
Composition of crude petroleum. Refining and different types of petroleum products and their applications. Fractional Distillation (Principle and process). Cracking (Thermal and catalytic cracking). Reforming Petroleum and non-petroleum fuels (LPG. CNG. LNG. bio-gas. fuels derived from biomass). fuel from waste. synthetic fuels (gaseous and liquids). clean fuels. Petrochemicals: Vinyl acetate. Propylene oxide. Isoprene. Butadiene. Toluene and its derivatives Xylene.

Petroleum is composed primarily of hydrocarbons, although hydrocarbon derivatives containing oxygen, nitrogen, or sulfur are also present. Additionally, some metals are present at trace levels. Different sources of petroleum exhibit different compositions, however the major hydrocarbon classes (alkanes [paraffins], cycloalkanes [naphthenes], and aromatics) are found in all sources of crude oil. Although the composition of crude oil varies from location to location, and even within a single well



Basic elemental composition of crude oil, which typically exhibits little variation from source to source

Ref.: https://www.sciencedirect.com/topics/chemistry/petroleum



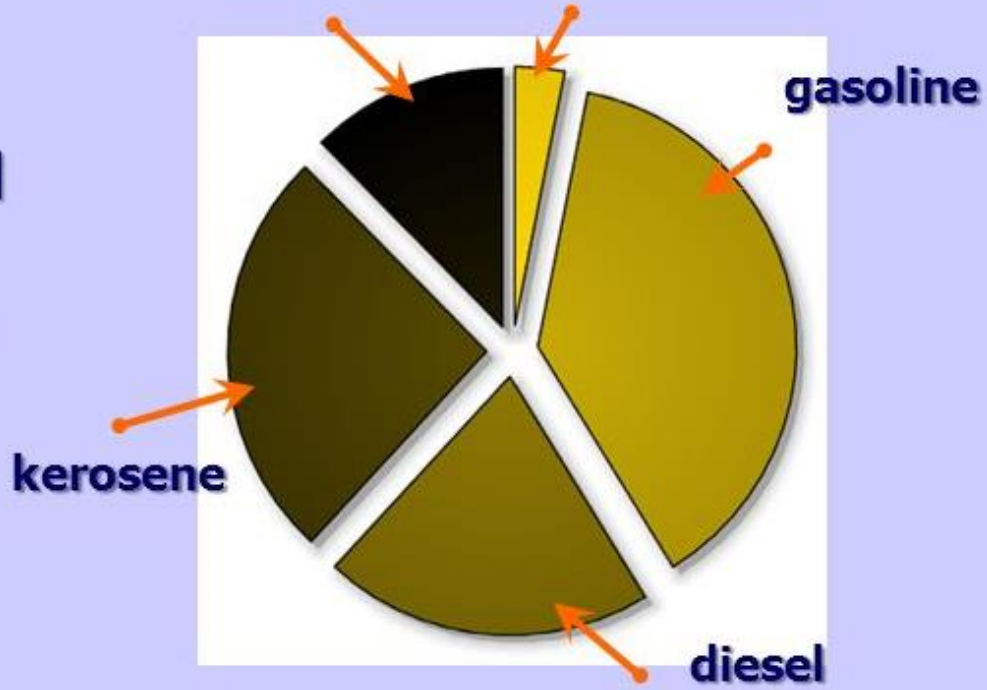
Composition of Crude Oil

Ref.: https://images.app.goo.gl/88kNf7CaG8p1VSgk7

Composition of Crude Oil

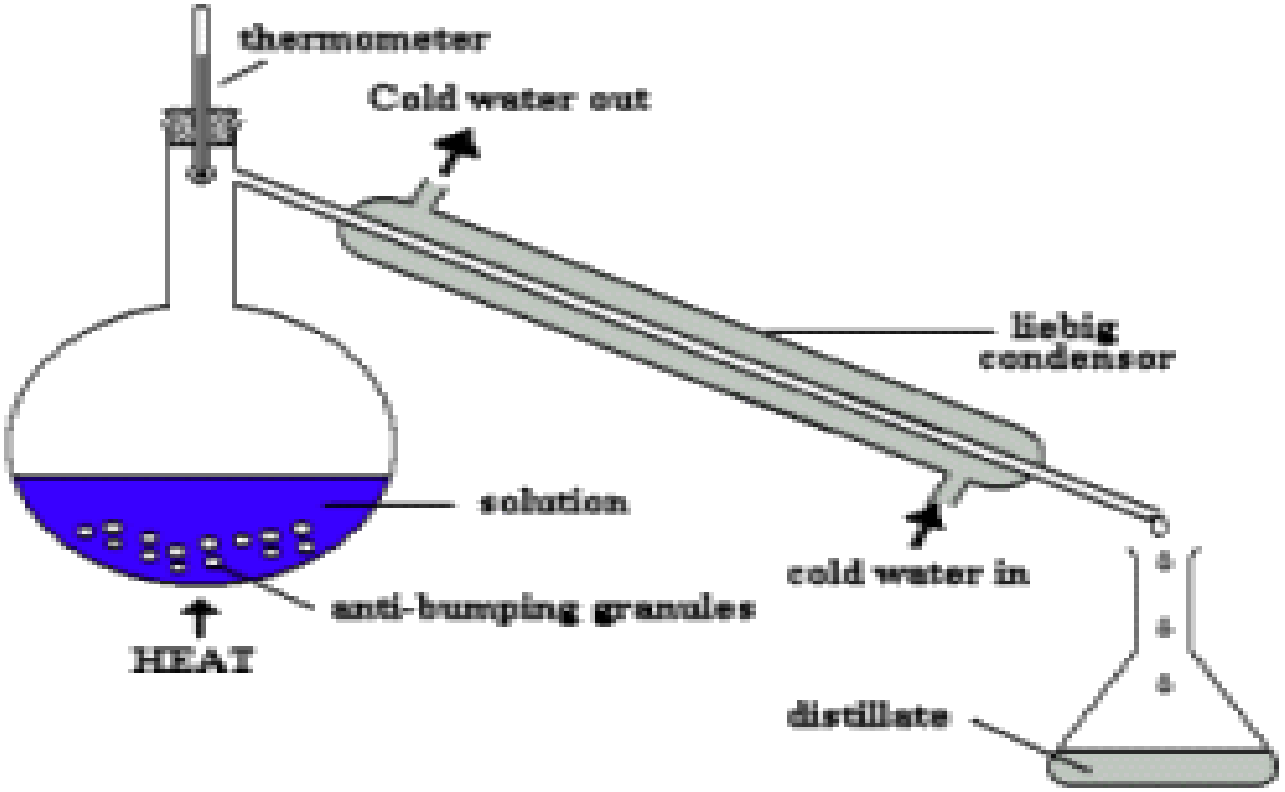
The exact composition of crude oil depends on where in the world the oil comes from.

Crude oil from the North Sea is a 'light' oil because it contains a large amount of small molecules and so a larger proportion of lighter fractions.



Crude oil from Saudi Arabia is a 'heavy' oil because it contains a large amount of large molecules and so a larger proportion of heavier fractions.

Principle of Distillation

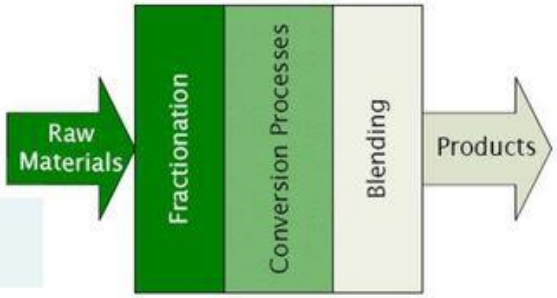


Ref. : www.google.com

The refining process

Every refinery begins with the separation of crude oil into different fractions by distillation.

❖ The fractions are further treated to convert them into mixtures of more useful saleable products by various methods such as;



- ❑ Cracking
- ❑ Reforming
- ❑ Alkylation
- ❑ Polymerisation
- ❑ Isomerisation

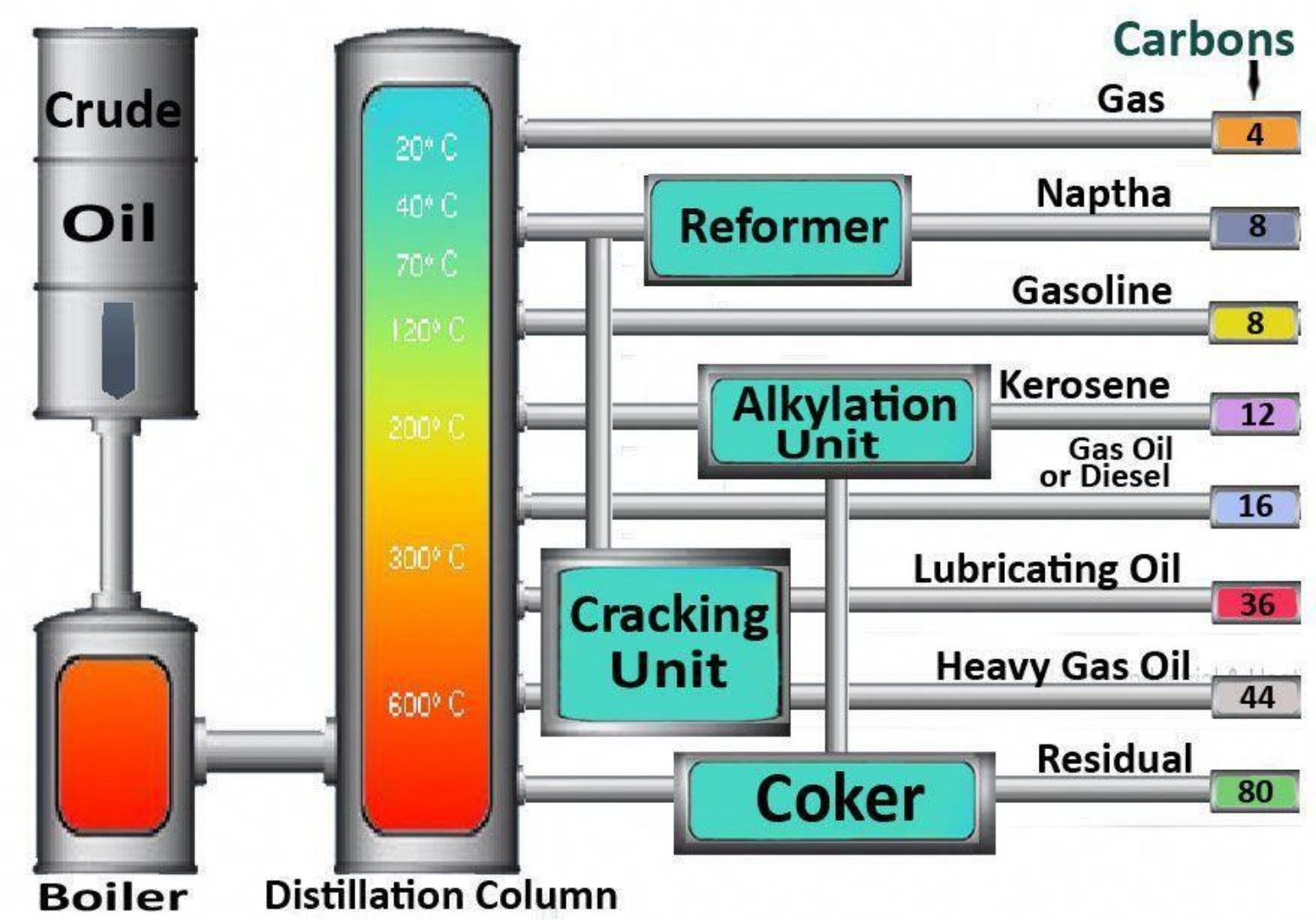
❖ These mixtures of new compounds are then separated using methods such as;

- ❑ Fractionation
- ❑ Solvent extraction

❖ Impurities are removed by various methods, e.g.

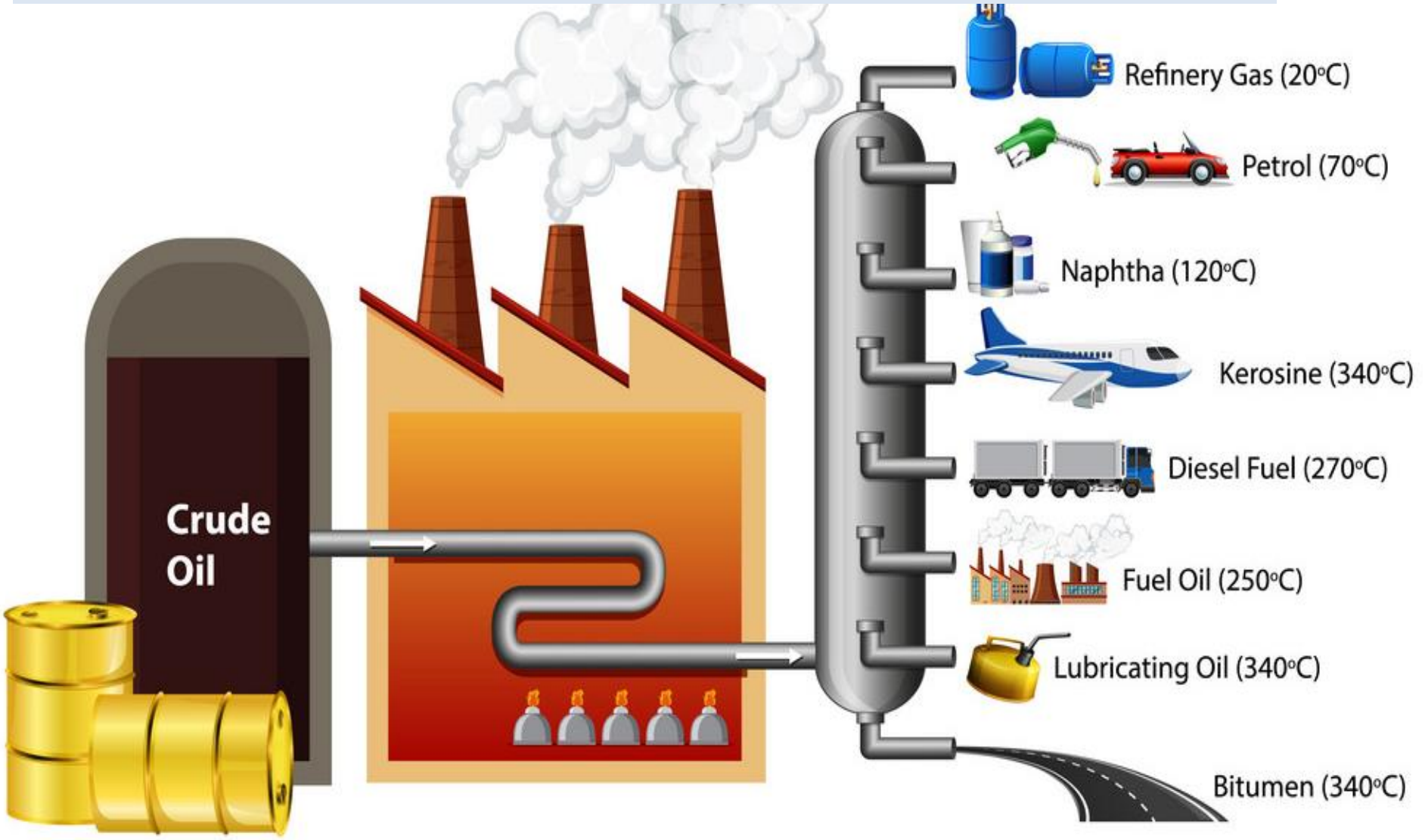
- ❑ Dehydration
- ❑ Desalting
- ❑ Sulphur removal
- ❑ Hydrotreating

Refining Process



Ref.: https://images.app.goo.gl/kXdvbnoQ4DRV7jDg6

Uses of the Petroleum Compound extracted from Crude Oil

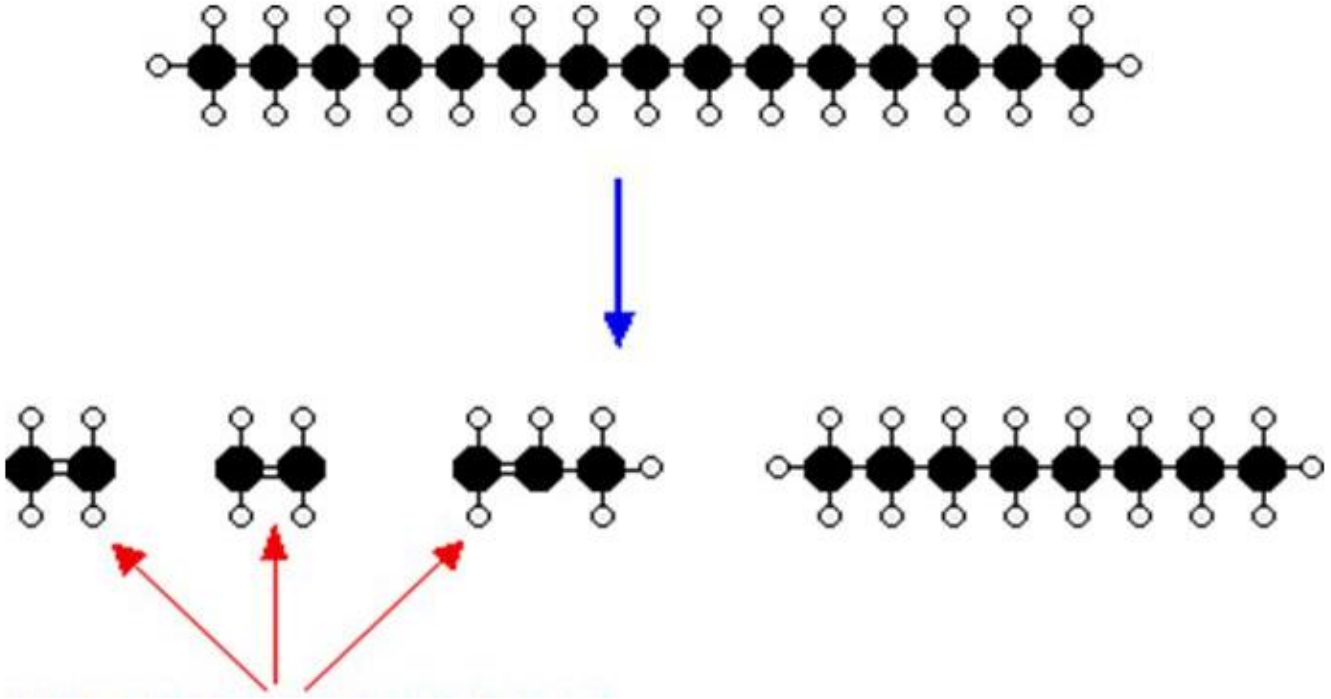


Cracking

Cracking involves longer chain hydrocarbons being broken up into shorter chain hydrocarbon.

$C_{15}H_{32} \longrightarrow 2C_2H_4 + C_3H_6 + C_8H_{18}$

ethene propene octane



Notice the double bond formed

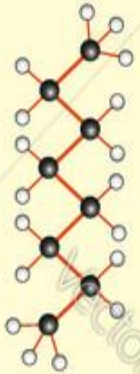
Importance of cracking

- **Producing extra petrol**
- High boiling fractions of C_{13} to C_{25} are cracked into small molecules which are fuels for motor-cars.
- **As a source of alkenes (raw materials for plastics)**
- Alkenes – by products of cracking and raw materials for making plastics, polymers and detergents.

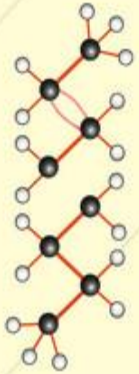
CRACKING PROCESSING

THERMAL

t = 480 - 550°C
P = 5 mPa

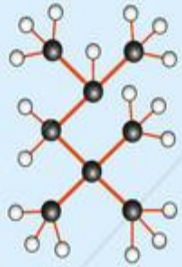


O.N. = 0

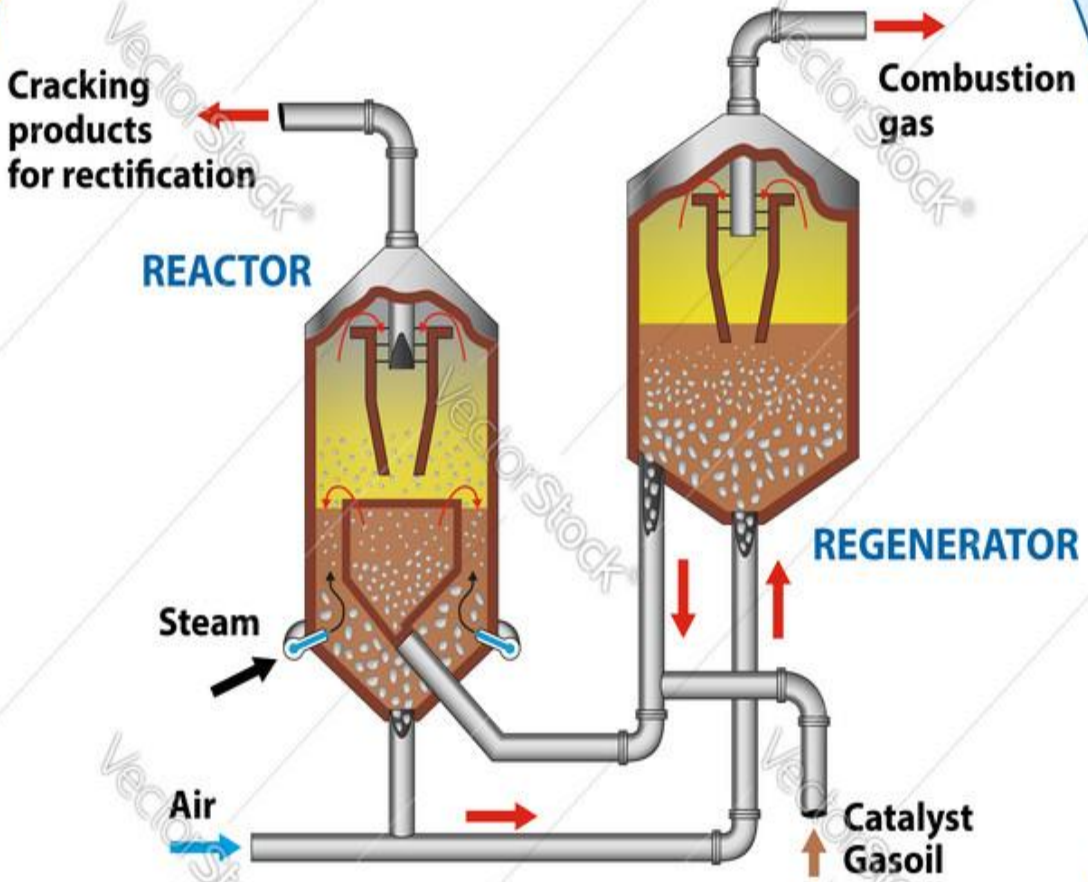


CATALYTIC

t = 450 - 500°C
$Al_2O_3 \cdot SiO_2$

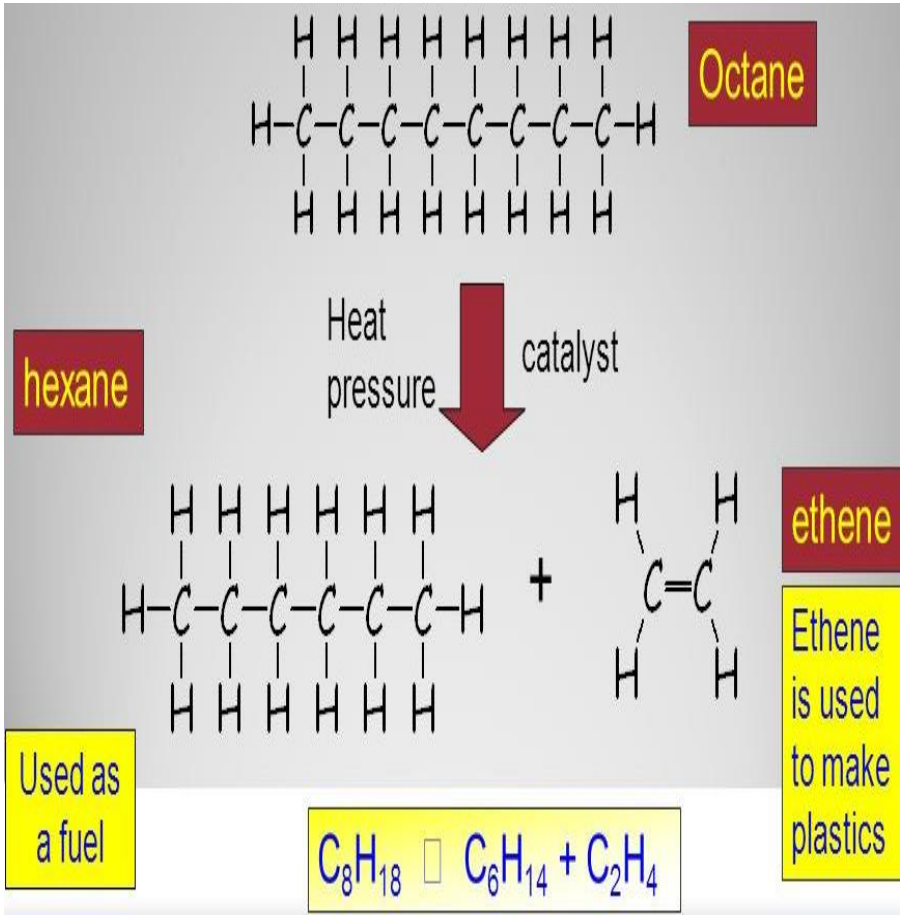


O.N. = 100

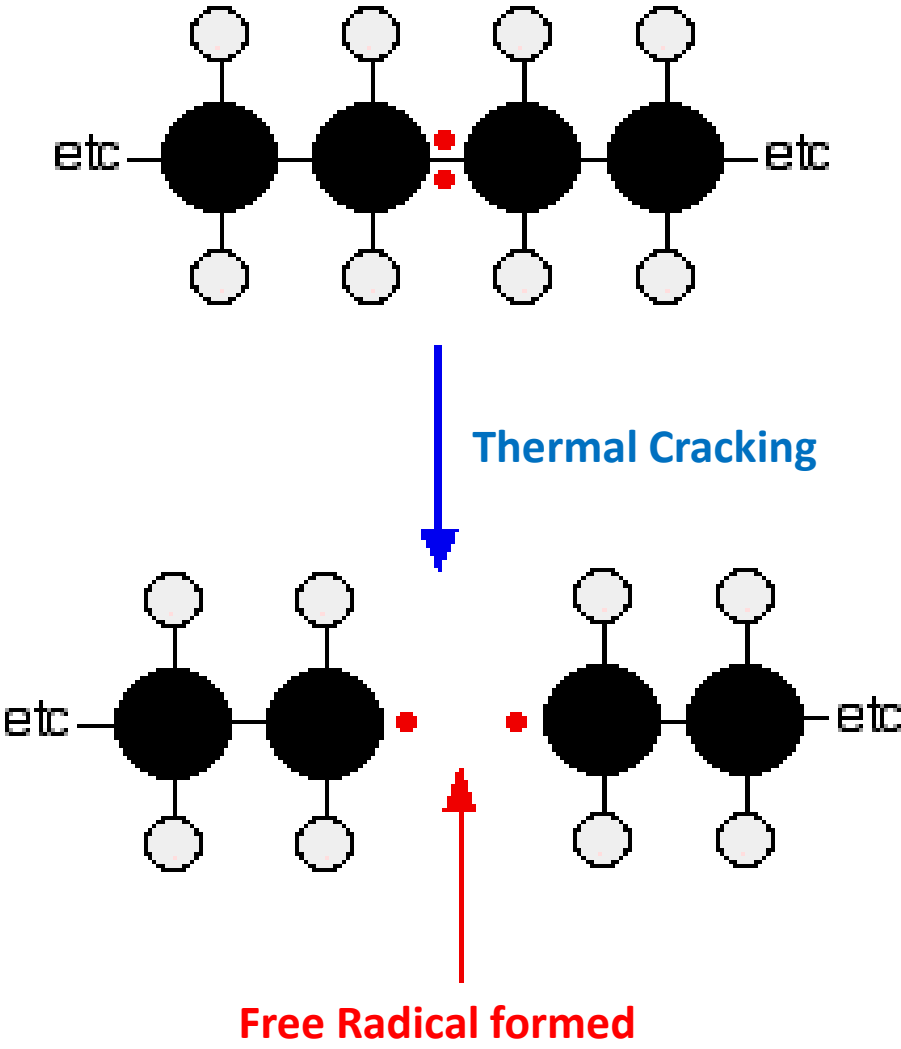


$$C_{16}H_{34} \longrightarrow C_8H_{18} + C_8H_{16}$$

Catalytic Cracking



Thermal Cracking



Thermal Cracking vs Catalytic Cracking

Thermal Cracking	Catalytic Cracking
Thermal cracking is the process of breaking down large compounds into small compounds at high temperatures and high pressures	Catalytic cracking is the breakdown of large compounds into small hydrocarbons using an acid catalyst
Involves cracking by applying high temperatures and pressures	Involves cracking by adding catalysts along with moderate temperature and pressures
The temperature ranges between 500-700 degrees Celsius	The temperature ranges between 475-530 degrees Celsius
Pressure used is about 70 atm	Pressure used is about 20 atm
Used for visbreaking, thermal gasoline production, and delayed coking	Used to obtain fuel with octane number 65-70

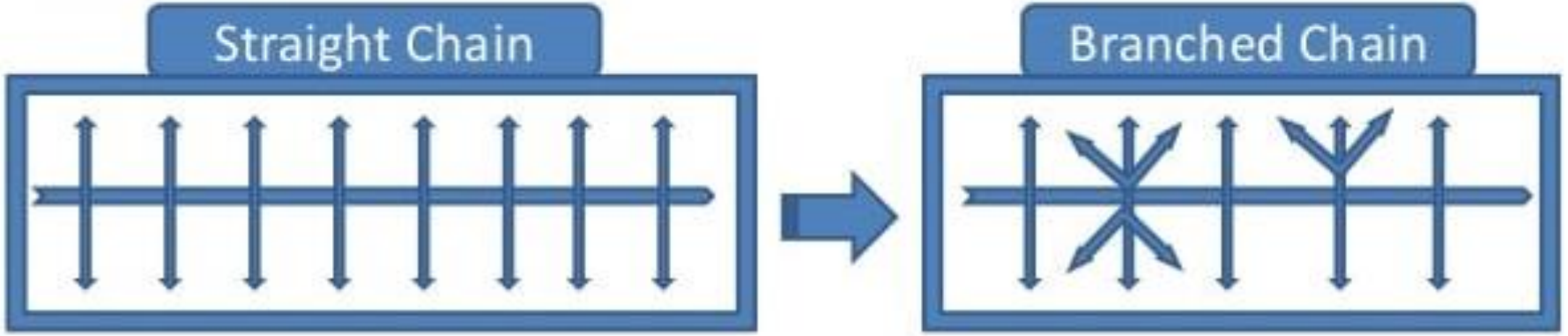
Fractional Distillation Vs Cracking

Fractional Distillation	Cracking
Fractional distillation is the process used to separate components in crude oil	Cracking is the process used to breakdown large hydrocarbon molecules into small hydrocarbons
Uses the difference between boiling points of components in a mixture	Involves the production of small hydrocarbons to improve the octane rating
Does not use catalysts	Can be done in the presence of catalysts
Depends on the boiling points of hydrocarbons in crude oil	Does not depend on the boiling points of hydrocarbons

Reforming of Petroleum

The word Reforms Means To **Recreate**

Reforming is a Process Which We Used to Better the Quality Of Petrol Or Diesel



Reform process Increase the **Octane Number** Of Gasoline or petrol

Octane Number is a standard measure of the performance of an **Engine** or **Fuel** .

Why we reform the petrol and Diesel

The Fuel Which We Get From **Refine Process** causes **Fuel Knocking**

Fuel Knocking High Frequency Vibrations giving rise to ping like sound inside an Engine

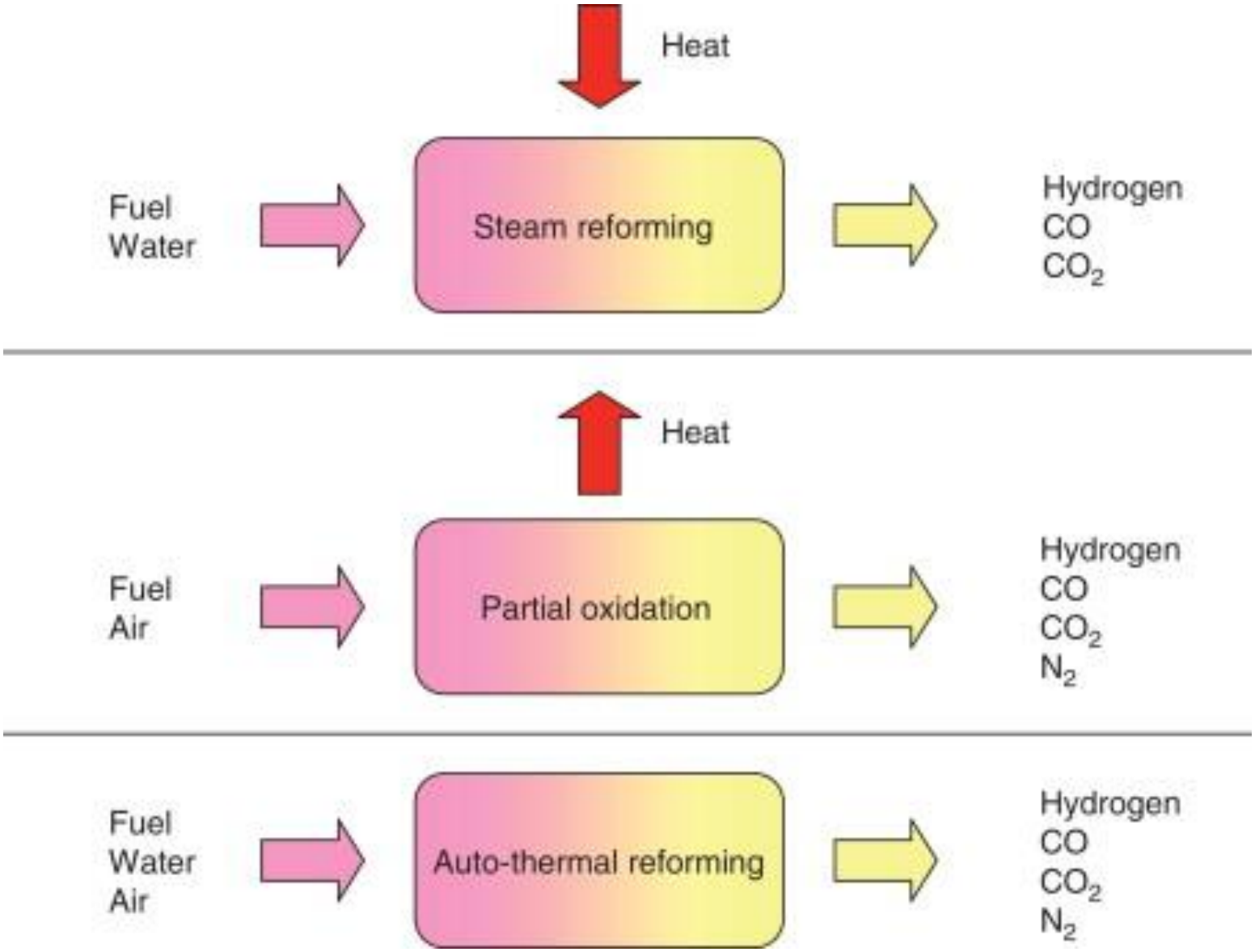
Mechanism of Reform Process

N-Octane

SiO_2

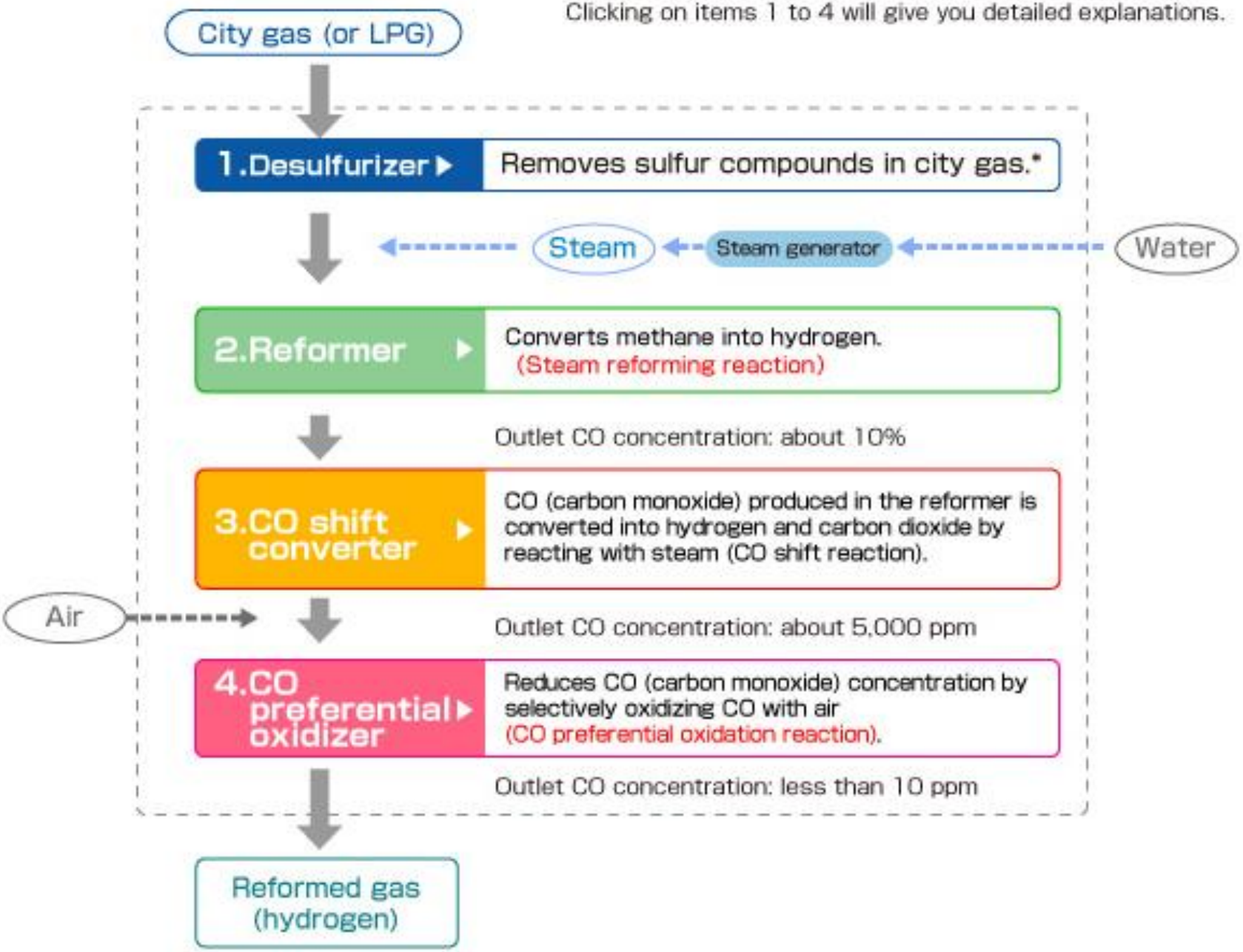
2,2,4-Trimethyl Pentane

Reforming Processes



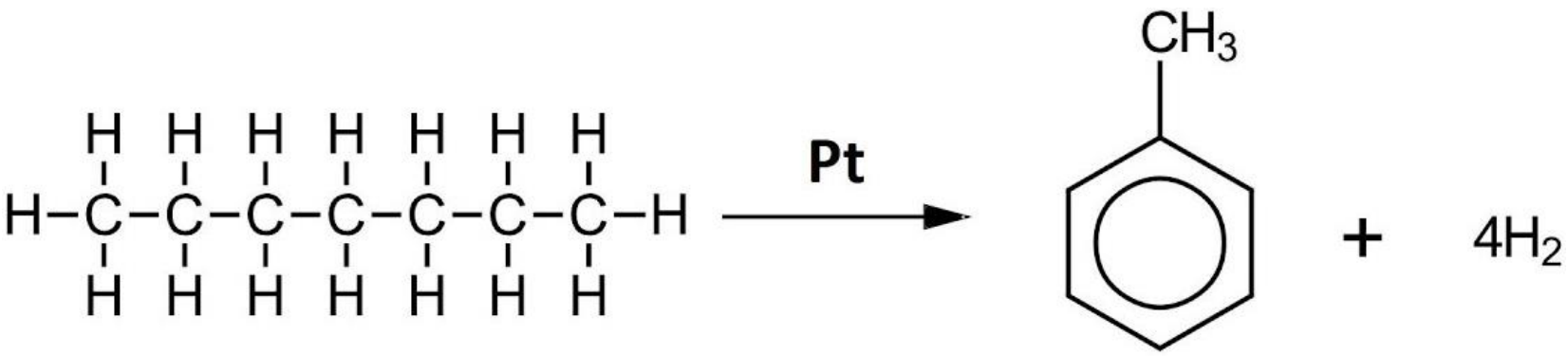
Process flow of natural gas fuel processing system

Clicking on items 1 to 4 will give you detailed explanations.



Catalytic Reforming

Deduce the equation for the conversion of heptane (C_7H_{16}) to methylbenzene ($C_6H_5CH_3$).



$$C_7H_{16} \rightarrow C_6H_5CH_3 + 4H_2$$

Catalytic Cracking Vs Catalytic Reforming

Catalytic Cracking	Catalytic Reforming
Catalytic cracking is the breakdown of large compounds into small hydrocarbons in the presence of a catalyst	Catalytic reforming is the process of converting low octane naphtha into high-octane reformate products
Most commonly used catalyst is Zeolite	Most commonly used catalysts are Platinum or Rhenium on a silica base
Includes the breakdown of larger hydrocarbons into smaller hydrocarbons	Includes the rearrangement of hydrocarbons in order to form different products
Feed is distillates obtained from crude oil distillation	Feed is naphtha feedstock
Mainly gives small alkanes and alkenes	Mainly gives isomerized and aromatic products

Synthetic Fuel Definitions

Synthetic Feed Stocks

Any feedstock not produced from conventional crude petroleum

Synthetic Fuels

A generic name given to hydrocarbon fuels produced from natural gas, coal or biomass

Recourses can be any burnable material:

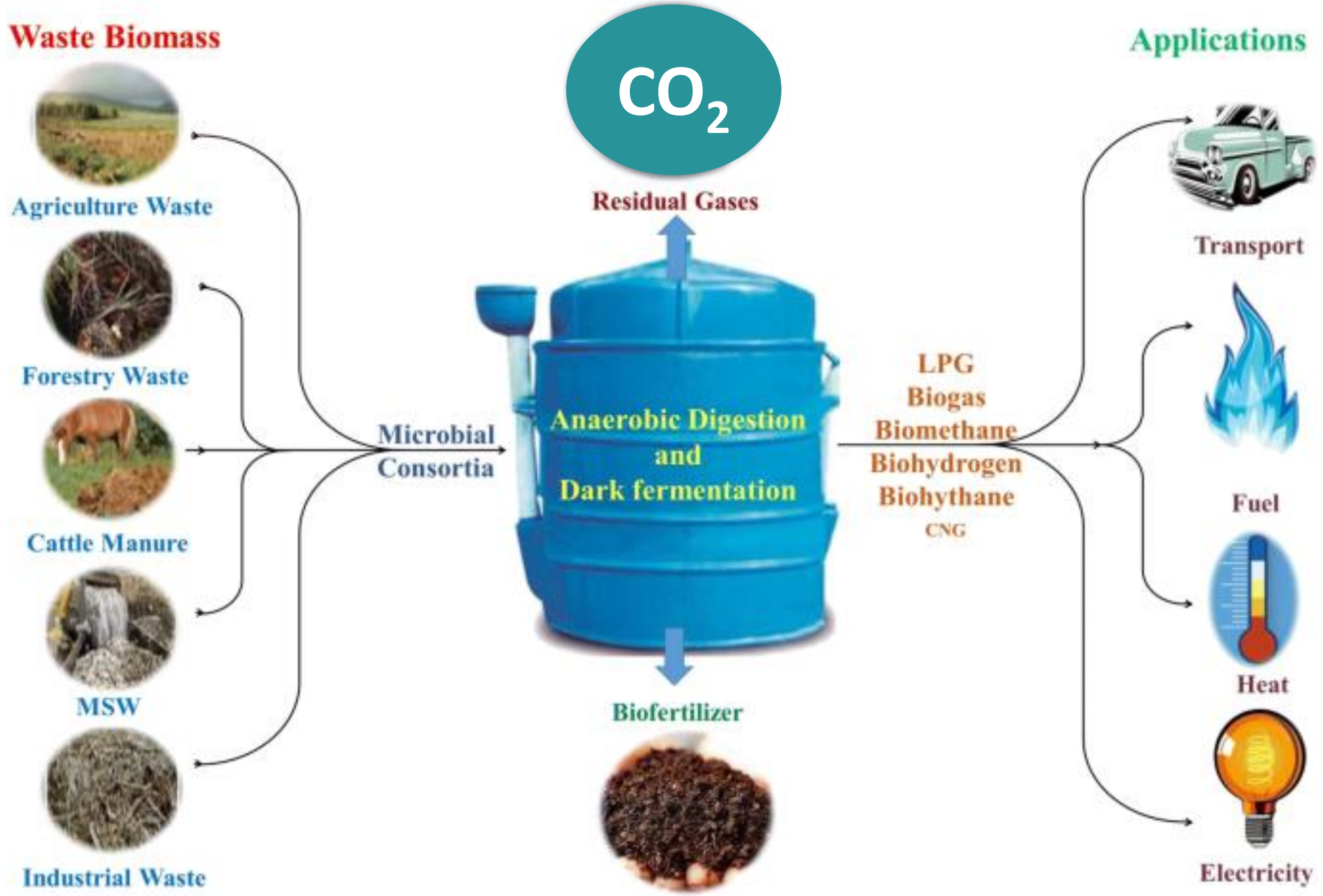
Coal
Biomass
Natural gas

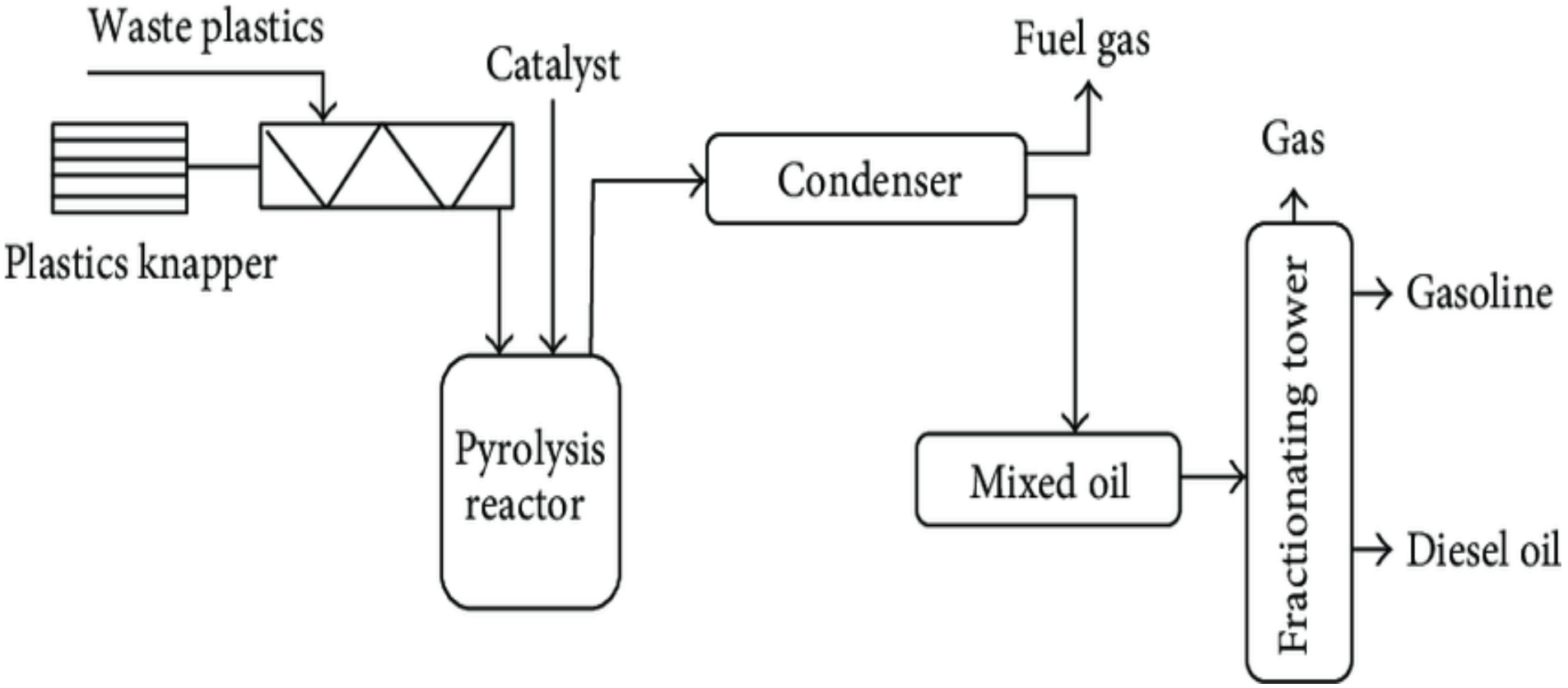
Necessity of Synthetic Fuels

5 Reasons for continued production and improvement of synthetic fuels.

- World has a finite supply of conventional crude oil.
- India's demand for crude oil is steadily increasing.
- The world jet fuel market is decreasing.
- Natural Security and energy independence.
- Synthetic Fuel help India to reduce dependency on foreign oil.

Fuel from Waste Material





Pyrolysis Process of generating fuel oil from the waste plastics

What is a clean fuel?

A Clean fuel is one which

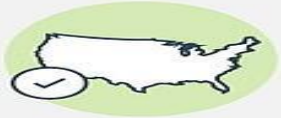
- When used, does not produce a polluting by product
- When processed, does not produce a polluting by product
- When processed or used, the by products are considered harmless

Examples of clean fuels include

- Hydrogen, in which its use produces waste water
- Solar Power, in which its use produces excess heat
- Hydropower, where the use has no by products
- Wind power, where the use has no by products

Benefits of Clean Fuels

1



Energy Security

2

Fuel Performance

3

Safety and Public Health

4

Emergency Support

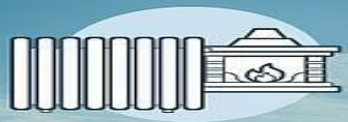
5

Safe and Dependable Storage

6

Cost Savings

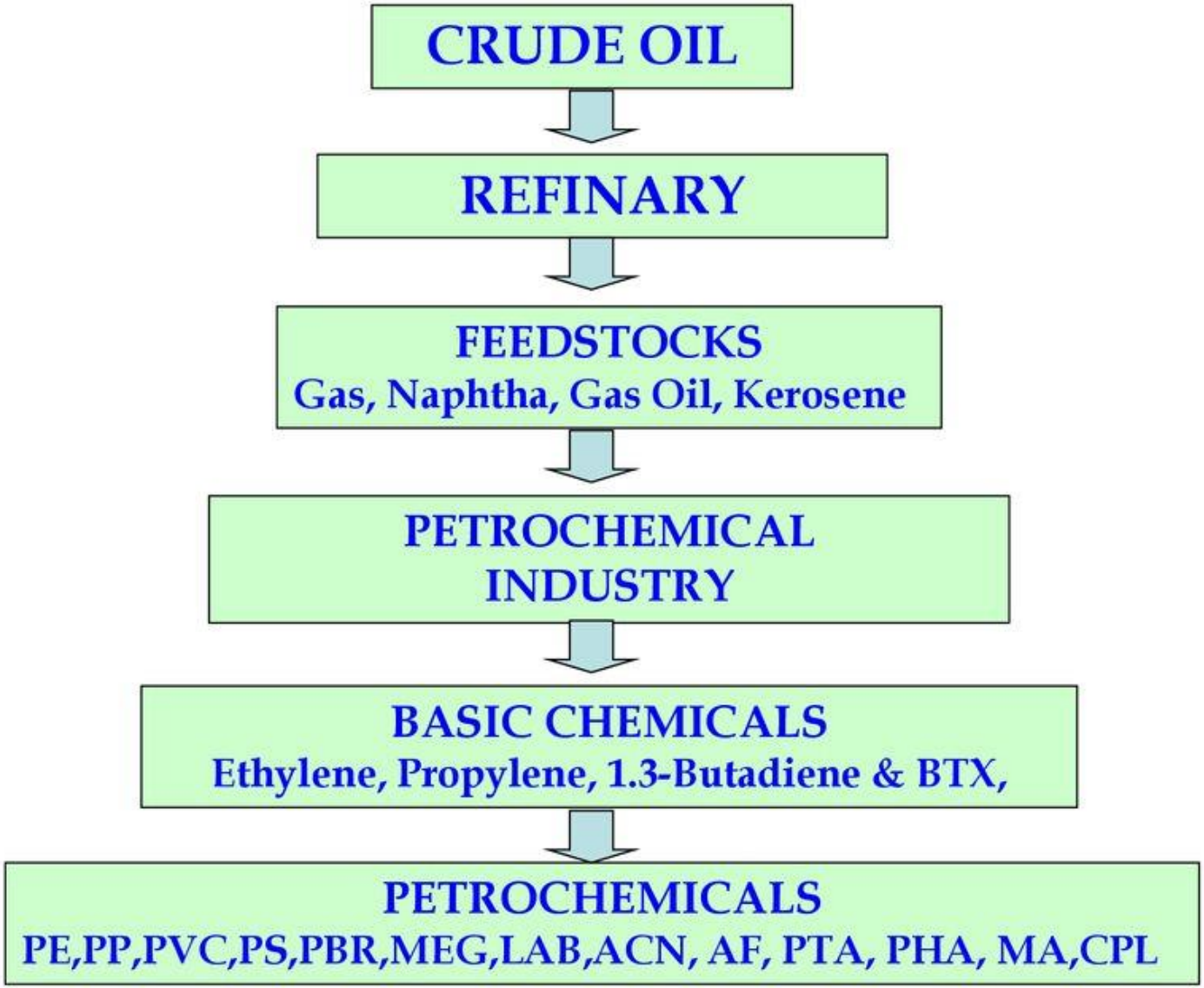
7



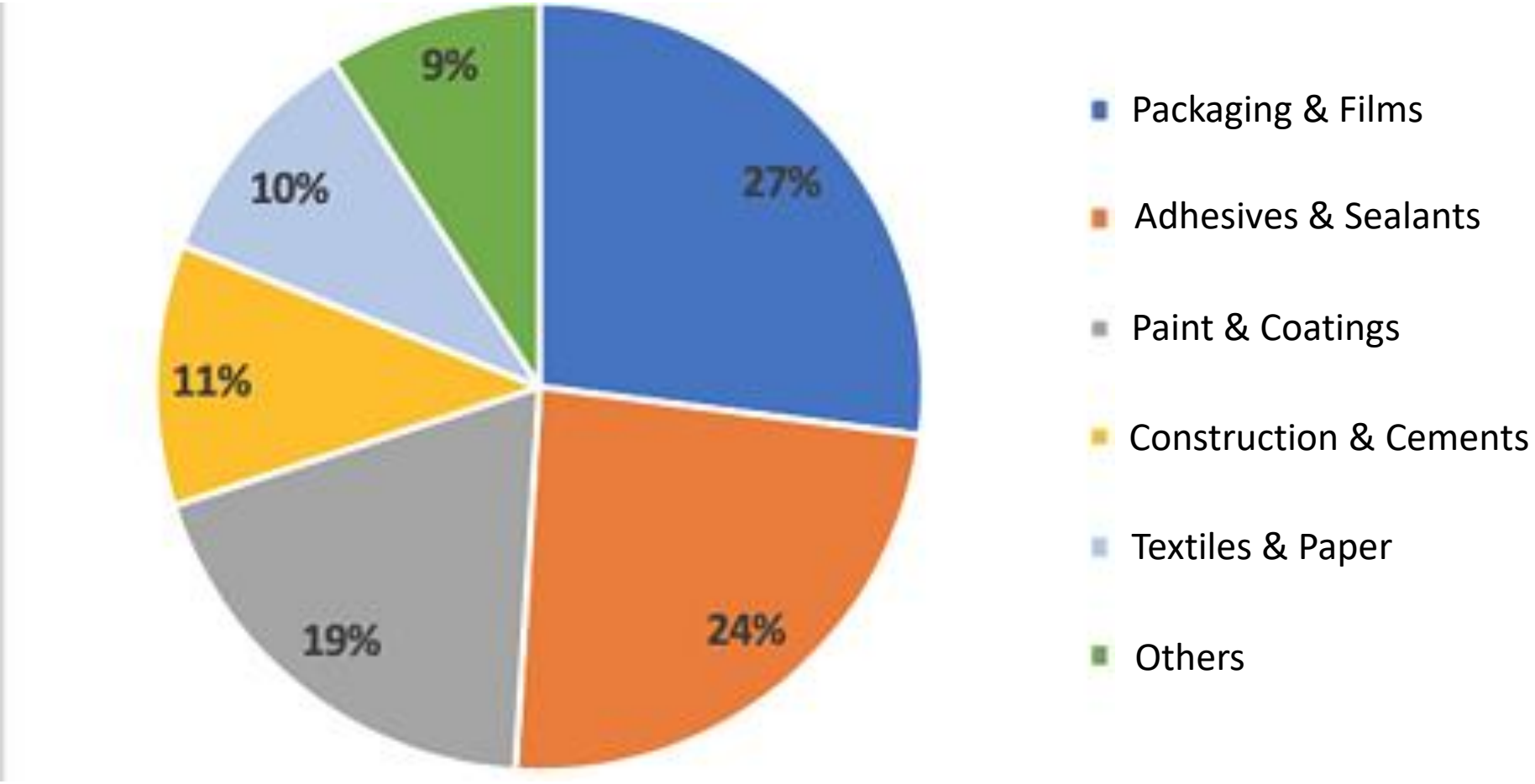
Immense Versatility

SmartTouch Energy®

Petrochemicals- The Origin



Global Vinyl Acetate Resin Applications, 2019



Advantages of Vinyl Acetate:

- Adhesion
- Chemical Resistance
- Clarity
- Oxygen Barrier
- Toughness

Propylene Oxide

- Colourless liquid, ether-like odour
- Dangerous product
- 3rd largest derivative of propylene
- Used as chemical intermediate in production of polyurethane polyols
- Used in manufacture of propylene glycol
- Manufactured by Dow, Lyondell and Shell Chemicals

Physical and chemical properties of propylene oxide

- **Physical Properties:**

  Propylene oxide is a colorless, highly volatile liquid at room temperature and normal atmospheric pressure.

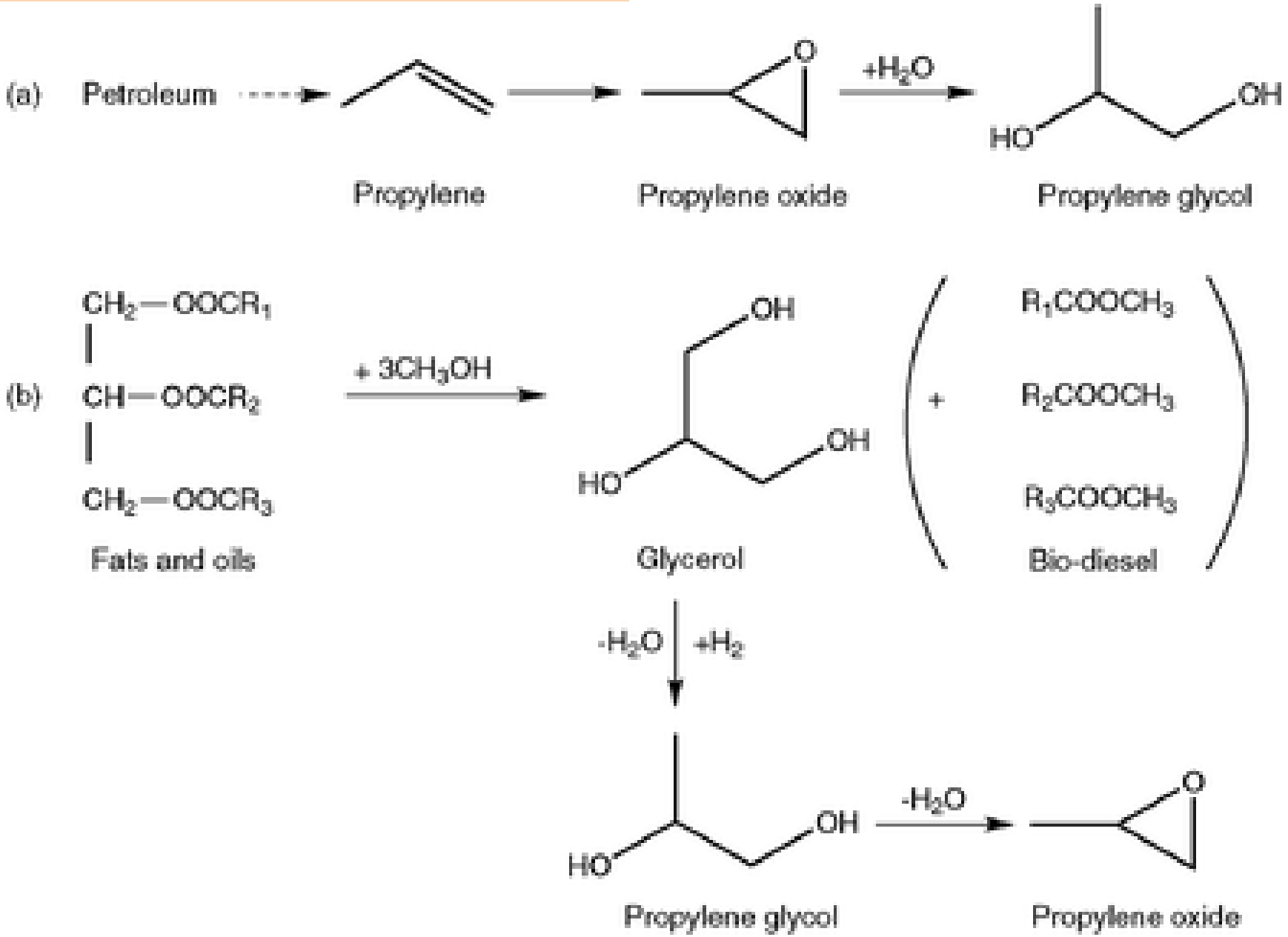
- **Chemical Properties:**

  Propylene oxide is a chemical compound that contains hydrocarbons and oxygen.

  Propylene oxide liquid is highly flammable and the vapor forms an explosive mixture with air.

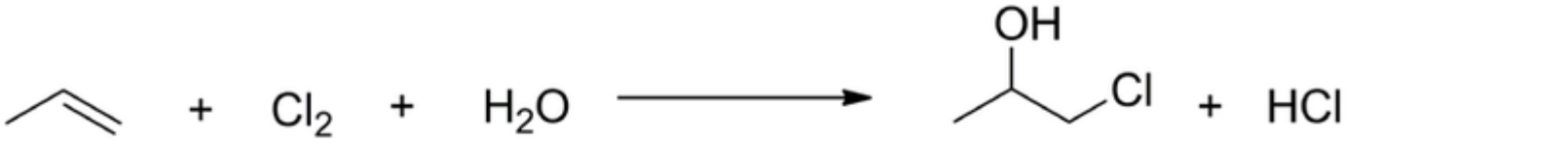
  Propylene oxide may polymerize violently. It is very reactive, particularly with chlorine, ammonia, strong oxidizing agents, and acids.

Propylene Oxide Synthesis



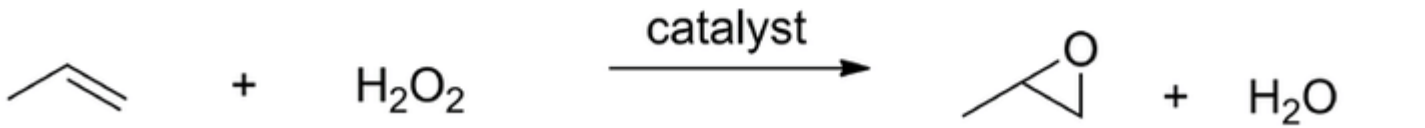
Propylene Oxide Synthesis

a. Chlorohydrin process:



25% atom economy

b. Catalytic epoxidation with H_2O_2:

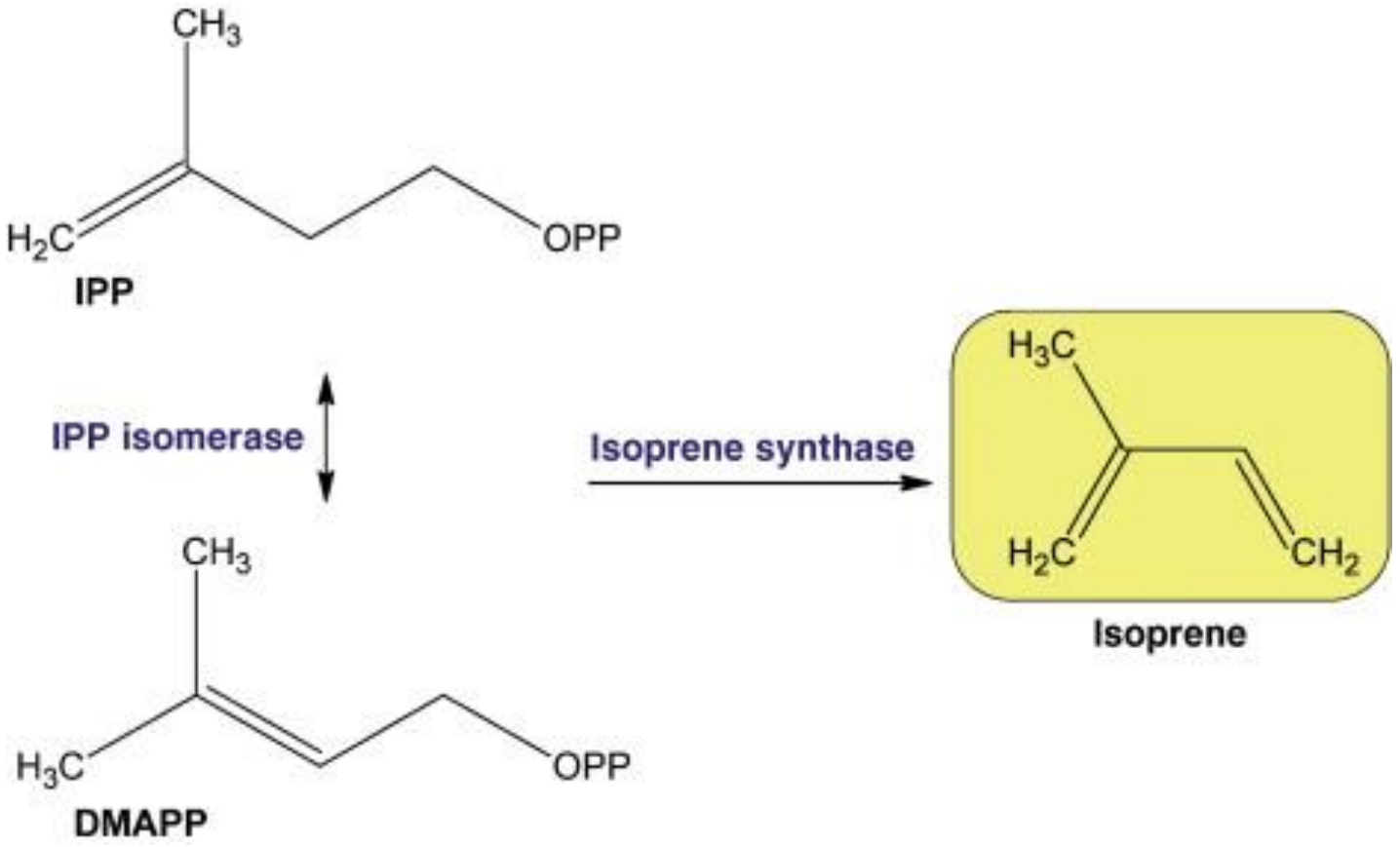


76% atom economy

Uses of Propylene Oxide

- PO is an important basic chemical intermediate.Virtually all the PO produced is converted into derivatives, often for applications similar to those of ethylene oxide (EO) derivatives.
- PO is used primarily to produce polyether polyols, propylene glycols, propylene glycol ethers and, and many other useful products.

Isoprene is a medium-value biochemical that is produced through steam cracking of oil. It is actually an important by-product of ethylene production and is almost entirely used for production of a synthetic substitute for natural rubber. It is also naturally produced by many plants as a heat stress response, where it was shown to increase the stability of photosynthetic membranes at high temperatures (Sharkey et al., 2001). It can represent as much as 2% of all carbon fixed by oak leaves at a temperature of 30 °C



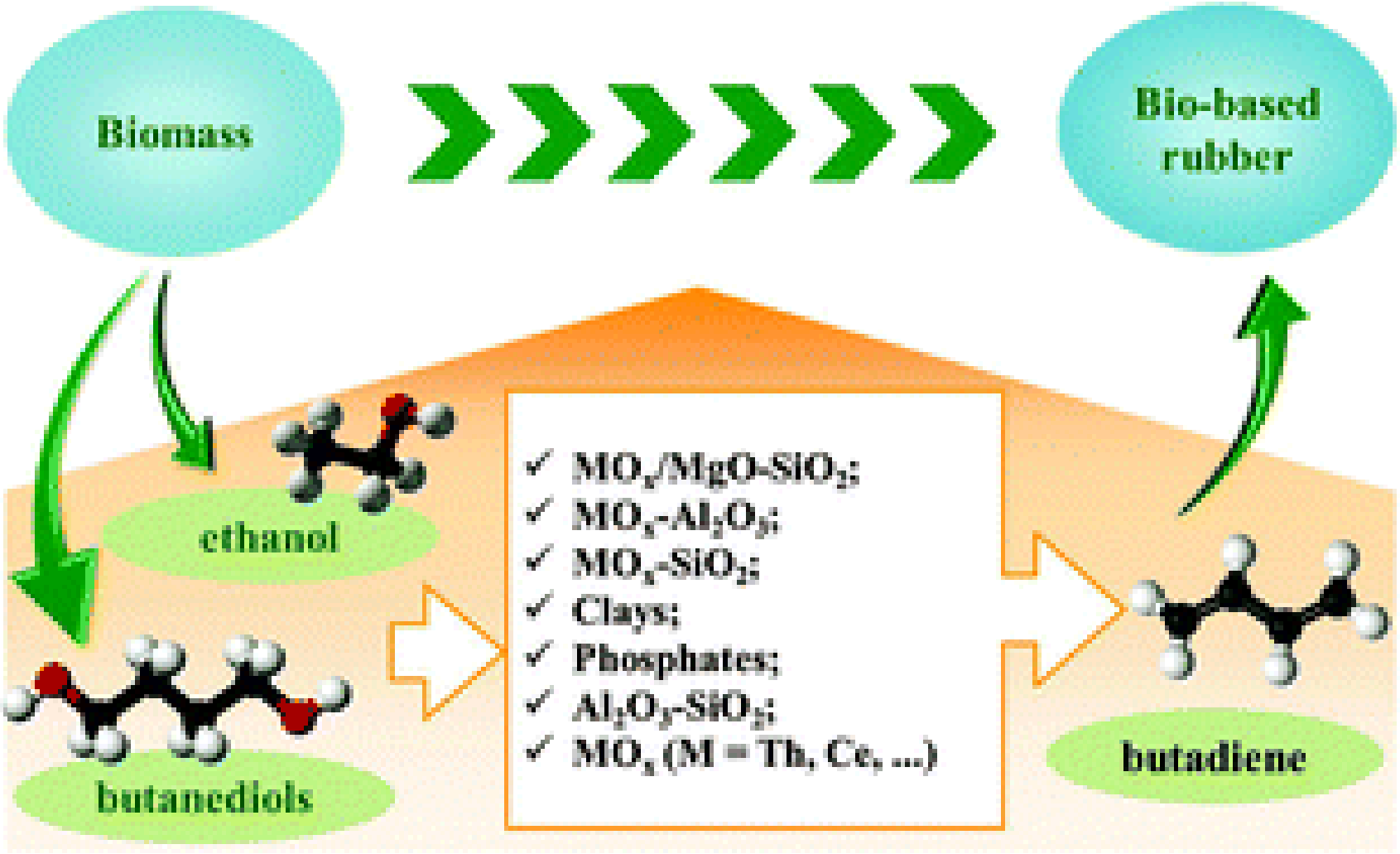
Uses of Isoprene

- This is derived from the sap of a tree
- It has a relatively high tensile strength
- Unfortunately solvents, petrol, mineral oils, and ozone readily attack it
- It degrades rapidly in the presence of strong sunlight
- Modified by additives to give it increased strength and wear resistant properties
- Natural rubber is used for vehicle tyres as it has excellent antiskid properties

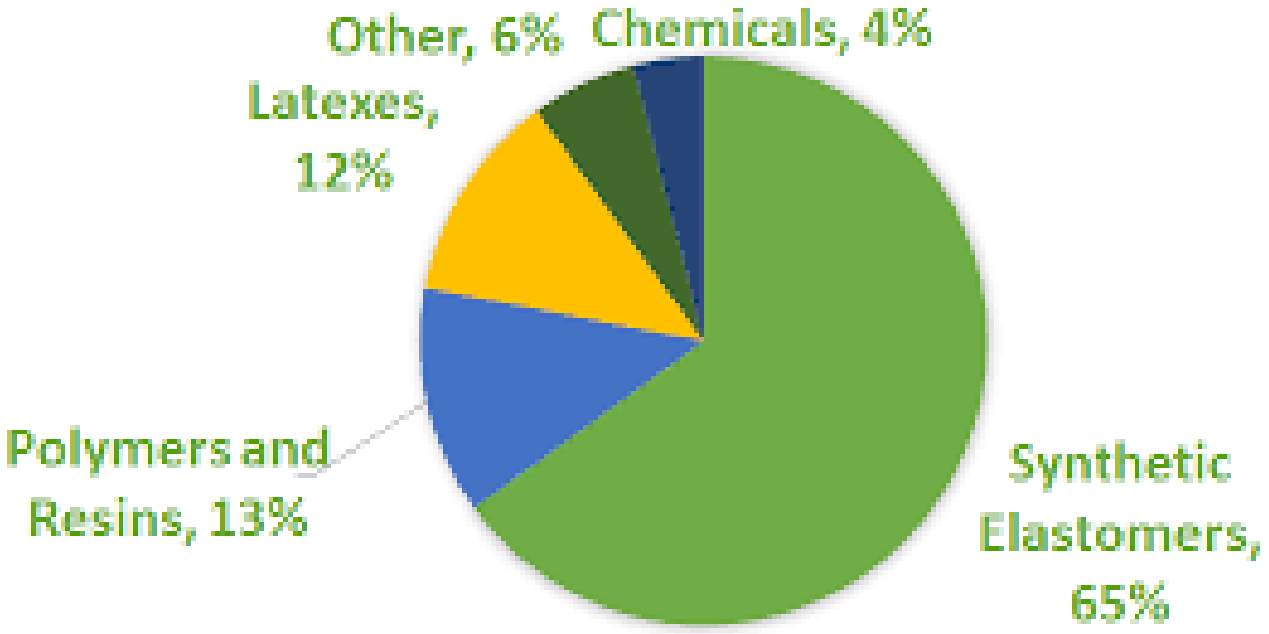
Uses of PolyIsoprene

- ✓Resistant to oxidizing agents and is damaged by aging, sunlight, oil.
- ✓Used in Domestic, textile, paper, carpet industry.
- ✓As adhesives, toy balloons, etc

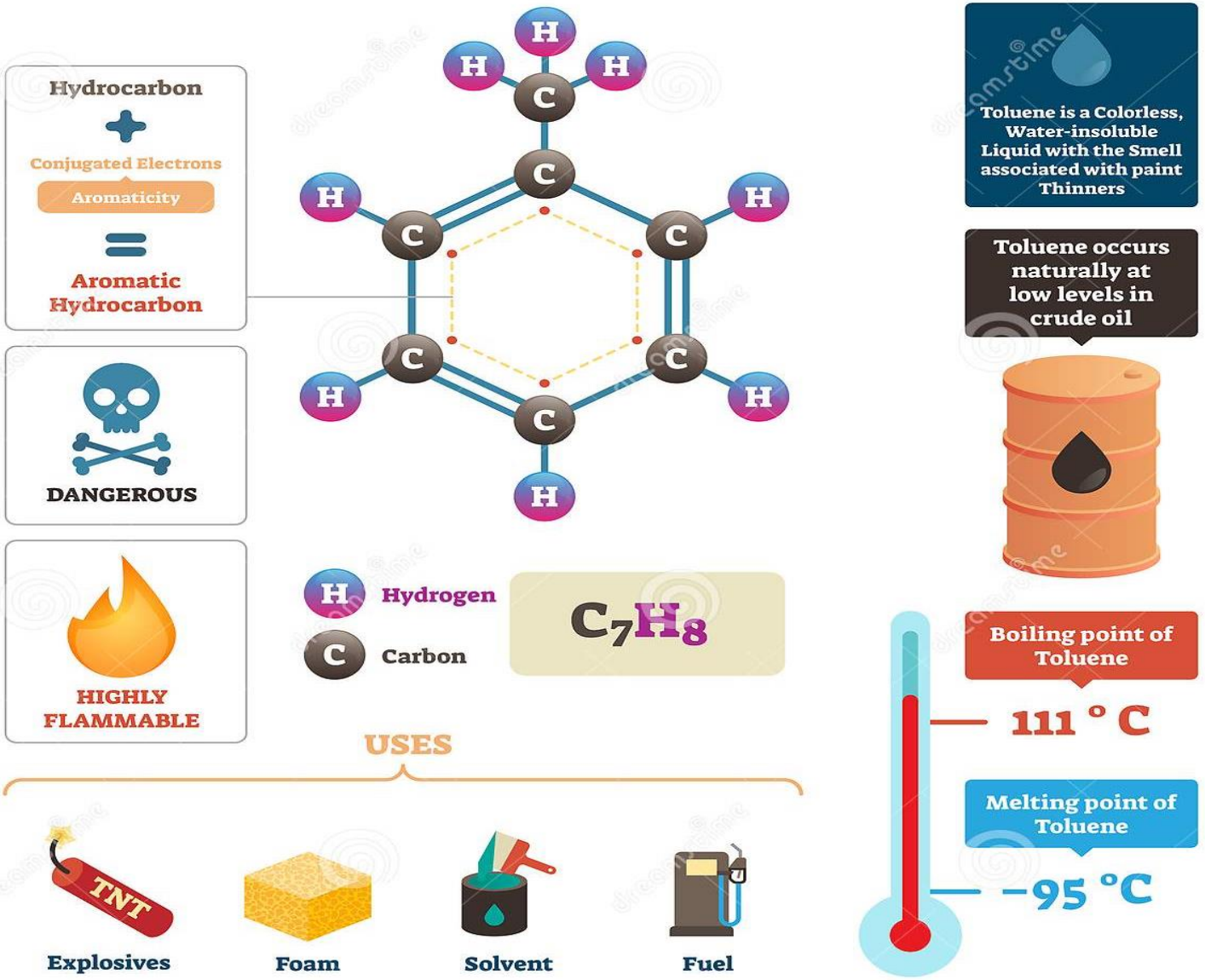
BUTADIENE


Biomass
Bio-based rubber
ethanol
butanediols
✓ $MO_x/MgO-SiO_2$;
✓ $MO_x-Al_2O_3$;
✓ MO_x-SiO_2;
✓ Clays;
✓ Phosphates;
✓ $Al_2O_3-SiO_2$;
✓ MO_x (M = Th, Ce, ...)
butadiene

BUTADIENE USE BY PRODUCT



TOLUENE


Hydrocarbon
Conjugated Electrons
Aromaticity
Aromatic Hydrocarbon
DANGEROUS
HIGHLY FLAMMABLE
H Hydrogen
C Carbon
C7H8
Toluene is a Colorless, Water-insoluble Liquid with the Smell associated with paint Thinners
Toluene occurs naturally at low levels in crude oil
Boiling point of Toluene
111 ° C
Melting point of Toluene
-95 °C
USES
TNT
Explosives
Foam
Solvent
Fuel

Origin of Xylene

- Xylene is origin include both naturally and manmade or synthetic method. It is widely used as a solvent in the leather, rubber, and printing industries. Other various applications of xylene include chemical intermediates, and high-motor and aviation gasoline blending agents, breathing devices (inhalers).

- Xylene is used in production of terephthalic acid monomer. It is a good cleaning agent for silicon wafers, steel and to sterilize many substances. Xylene is used as a feedstock in the production of petrol. It is also found in small proportions in gasoline and jet fuel.

Industrial Applications

- Toluene has numerous commercial and industrial applications and is a solvent in paints, lacquers, thinners, glues, correction fluid and nail polish remover
- Toluene used in the printing and leather tanning processes.
- Methylbenzene can also be used as a fullerene indicator, and is a raw material for toluene diisocyanate.

Xylene applications

- P-Xylene is the principal precursor to terephthalic acid and dimethyl terephthalate, both monomers used in the production of polyethylene terephthalate (PET) plastic bottles and polyester clothing.
- O-Xylene is an important precursor to phthalic anhydride.
- Xylene is substituted for toluene where slower drying is desired, and thus is used by conservators of art objects in solubility testing.
- It is used in the laboratory to make baths with dry ice to cool reaction vessels, and as a solvent to remove synthetic immersion oil from the microscope objective in light microscopy.
- In histology, xylene is the most widely used clearing agent.
- Xylene is used to remove paraffin from dried microscope slides prior to staining.


XYLENE
XYLENE


SRW
PRODUCTS
solid solutions to better hardscapes
XY
XYLENE
Specialty Clean™
XYLENE
SOLVENT
• Aids in Clean-up of Tools
• Removes Unwanted Overspray
• Dissolves and Thins Acrylic Sealers
DANGER! FLAMMABLE LIQUID AND VAPOR HARMFUL.
1 U.S. Quart (.95 Liters)

USE