

Content:

- **Engineering materials and Polymer Chemistry:** Glass, ceramics, refractory, composites, magnetic materials, Polymer, Properties, Polymer processing, Industrial polymers, conducting polymers
- **Natural Products and Biomolecules:** Amino acids/nucleic acids/proteins/lipids, Enzymes, Vitamins, Biomacromolecules, and Solid phase synthesis.
- **Fuels and Combustion:** Properties of fuels, Calorific value, Petroleum and petrochemicals, biofuels.
- **Electrochemical Systems:** Electrochemical cells and EMF, Applications of EMF measurements, Nernst Equation, Batteries, Fuel cell, corrosion and its control.

Textbook books:

1. P. Atkins and J. Paula, Physical Chemistry, 10th Edition, Oxford University Press, Oxford.
2. F. A. Cotton, and G. Wilkinson, Advanced Inorganic Chemistry, 5rd Ed., Wiley.
4. H.D. Gesser, Applied Chemistry - A Textbook for Engineers and Technologists, Springer

Reference books:

1. Fred W. Billmeyer, Text Book Polymer Science, Wiley India Pvt. Ltd.
2. D. J. Shriver, P. W. Atkins, and C. H. Langford, Inorganic Chemistry, 3rd Ed., ELBS.

Bomb calorimeter

❑ ***Formula for Higher Calorific Value (HCV) & Lower Calorific Value (LCV)***

$$\text{HHV} = 32,796 C + 141,886 (H - O / 8) + 9300 S \quad (\text{kJ/kg})$$

$$\text{LHV} = \text{HHV} - 2440(W + 9H) \quad (\text{kJ/kg})$$

- In these relations, the letters C, H, O, S, and W are percent weights of carbon, hydrogen, oxygen, sulfur, and water vapor in the coal composition, respectively.

Calorific value

❖ Lower and higher heating values of some fuels

Fuel type		Unit	Lower heating value		Higher heating value	
			kcal	kWh	kcal	kWh
Wood		kg	2500	2.90	2800	3.25
Coal	Lignite	kg	3000	3.50	3300	3.84
	Export	kg	6000	6.98	6500	6.96
Diesel		kg	10200	11.86	10,800	12.58
Natural gas		m ³	8250	9.59	9155	10.62
Heater fuel		kg	9700	11.28	10,500	12.18
LPG (30% propane, 70% butane)		m ³	26,000	30.16	28,200	32.71
		kg	11,000	12.76	11,900	13.80
Propane		m ³	21,200	23.95	23,000	25.93
		kg	11,100	12.87	12,000	13.98
Electric		kWh	860	1	860	1
Fuel oil		kg	9700	11.28	10,500	12.18

Calorific value

❖ Heating (calorific) values of some fuels

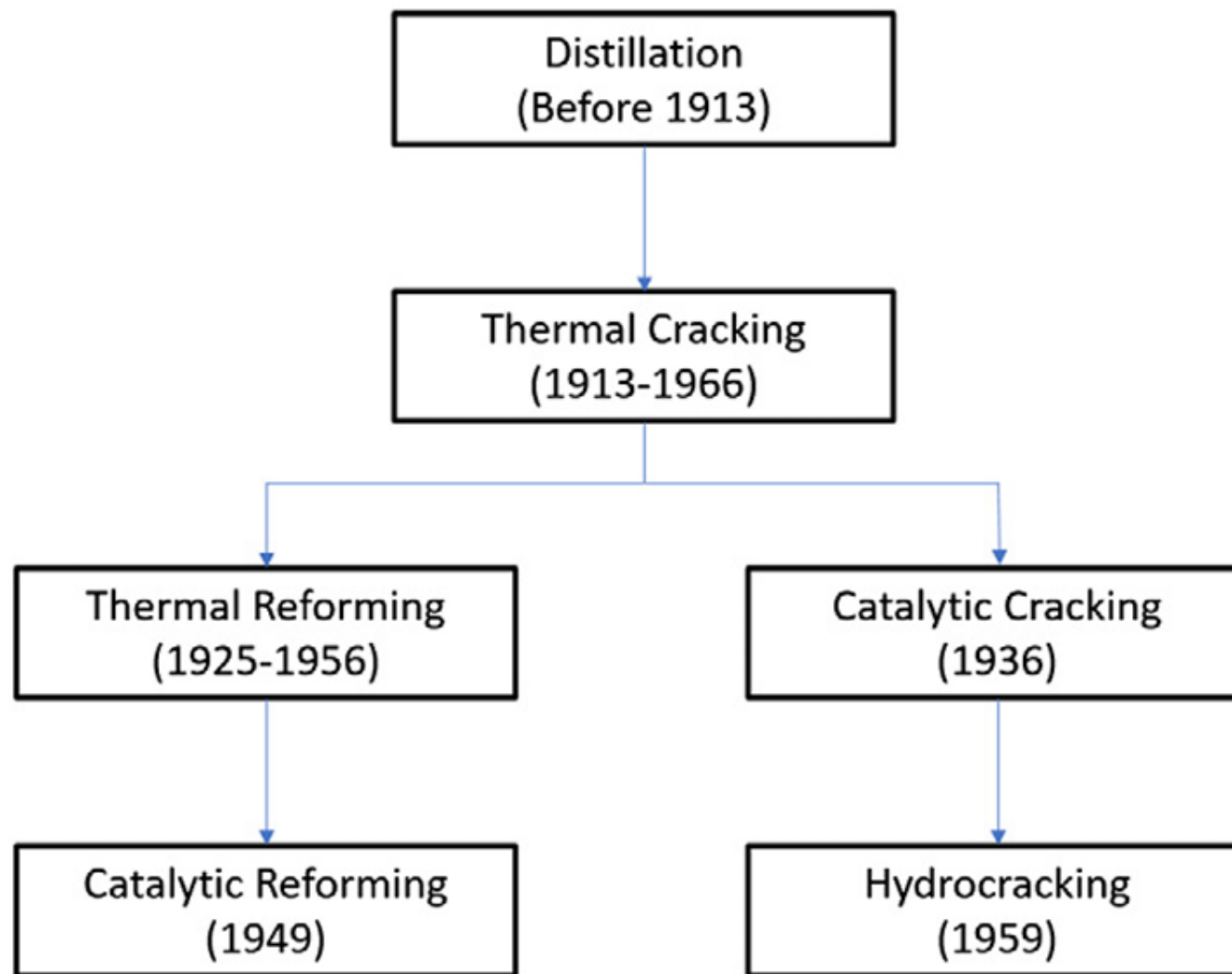
Fuel	Heating value (MJ/kg)	Fuel	Heating value (MJ/kg)
Animal/plant waste	9.62	Propane	42.70
Asphaltites	18.00	Fuel gas	43.96
Briquette	20.93	Acetylene	59.57
Coal	23.02	Coke gas	16.85
Coke dust (powder)	25.12	Natural gas	34.54
Crude oil	43.96	LPG	45.63
Graphite	33.49	Naphtha	43.54
Industrial lignite	12.56	Fuel oil No: 5	41.97
Lignite plant	8.37	Fuel oil No: 6	41.28
Petro-coke	31.81	Gasoline	43.54
Prina (Olive pomace)	18.00	Gas oil	34.70
Sawdust	12.56	Black liquor	12.56
Wood	12.56	Diesel fuel	42.70

The role of innovation and technology in sustaining the petroleum and petrochemical industry

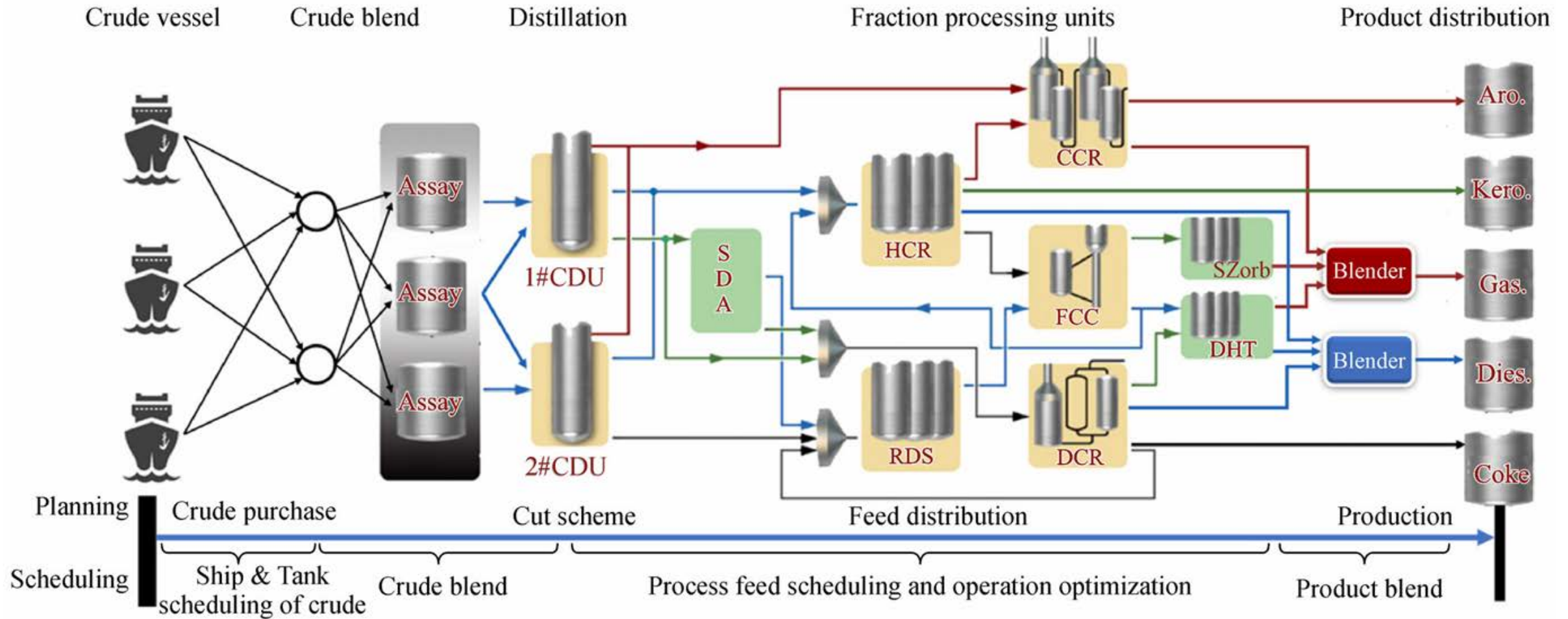
- ☐ Petroleum, the New “Black Gold”
- ☐ The word "petroleum" means "rock oil" or "oil from the earth" (EIA, 2005). Mankind has known petroleum or crude oil since the dawn of civilisation.
- ☐ It was used in ancient Persia and Burma, particularly as fuel for lamps. Burning of the natural gas (escaping from petroleum underground) gave the 'perpetual fire' at Baba Gurgur in Iraq (Arene and Kitwood, 1979).
- ☐ Innovation and Technology go hand in hand within the petroleum and petrochemical industry.
- ☐ Oil price volatility, geopolitics, and economic uncertainty, all contribute towards the continued need to innovate and technologically advance if petroleum and petrochemical companies are to survive in this highly competitive industry.
- ☐ Thereafter, the focus shifts towards identifying both quantifiable and non-quantifiable impacts of technology and innovation within the petroleum and petrochemical industry.



Historical innovations in petroleum refining processes



Production planning and scheduling optimization



The Origin of Petroleum

The formation of petroleum has long been debated, but two main theories are generally discussed:

❖ 1. Biogenic Theory (widely accepted):

- ❑ Petroleum originates from the slow decomposition of marine plant and animal remains, especially plankton, that settled in ancient seas.
- ❑ Over hundreds of millions of years, these organic deposits were buried under layers of mud and sand.
- ❑ With increasing temperature, pressure, and time, the organic matter was converted into kerogen (a waxy substance).
- ❑ Further thermal decomposition of kerogen produced liquid petroleum and natural gas.
- ❑ The petroleum then migrated through porous rocks until it became trapped beneath impermeable layers, forming oil and gas reservoirs.

❖ 2. Abiogenic or Atmospheric/Chemical Theory (minority view):

- ❑ Suggests that petroleum could have been generated by purely chemical processes within the Earth's mantle.
- ❑ Hydrocarbons might have been formed from carbon present in the early atmosphere and later trapped underground.
- ❑ This theory, however, faces challenges, especially in explaining how such petroleum could accumulate in the vast quantities found in commercial reservoirs.

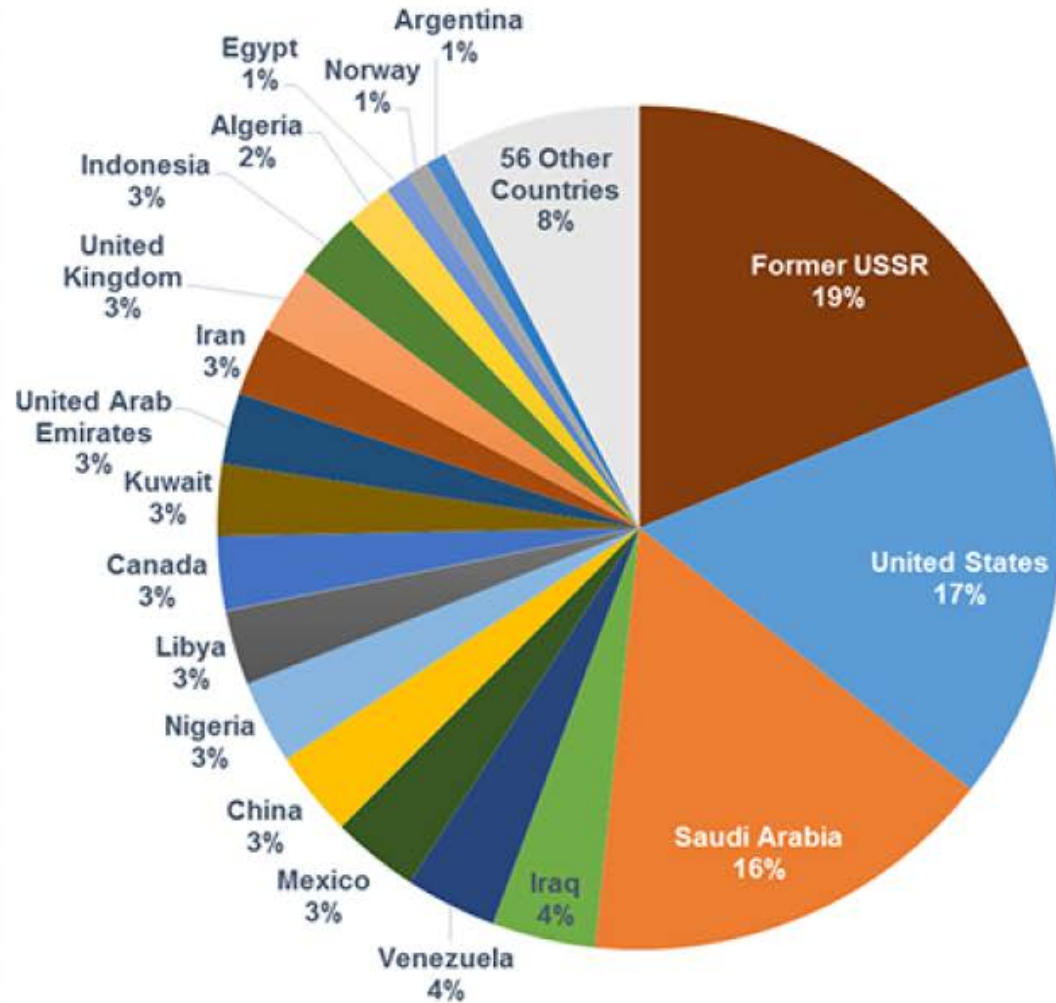


Petroleum Exploration

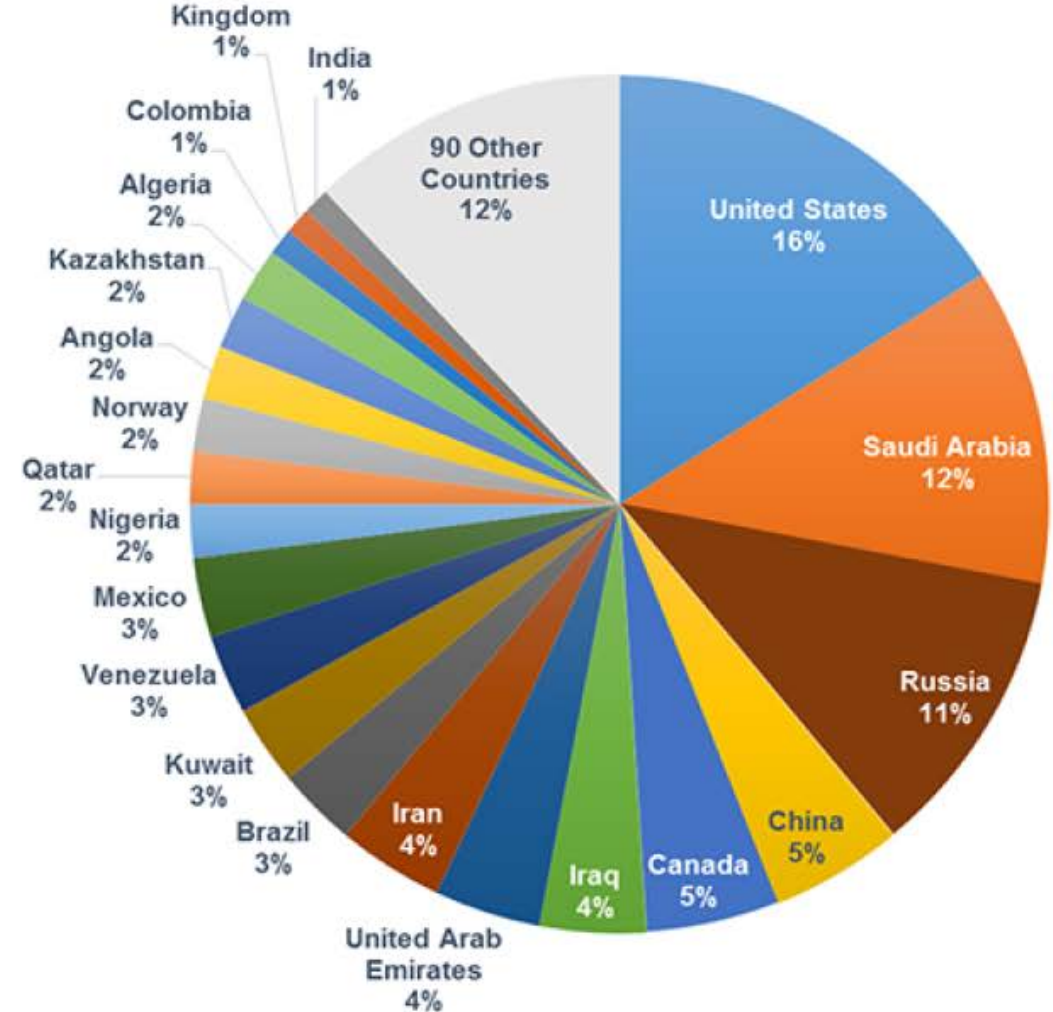
- ❑ Petroleum exploration is the process of locating underground oil and gas reserves.
- ❑ It requires specialized knowledge of geology, geophysics, and geochemistry to identify potential source rocks, reservoir rocks, and structural traps.
- ❑ Modern exploration techniques include:
 - ❑ Seismic surveys (2-D, 3-D, and even 4-D) to map subsurface structures.
 - ❑ Drilling exploratory wells to confirm the presence of hydrocarbons.
 - ❑ Geological modeling to estimate the size and quality of reserves.
- ❑ Successful exploration results in proven reserves, which can then be developed for commercial production.

Major Petroleum Producing Countries

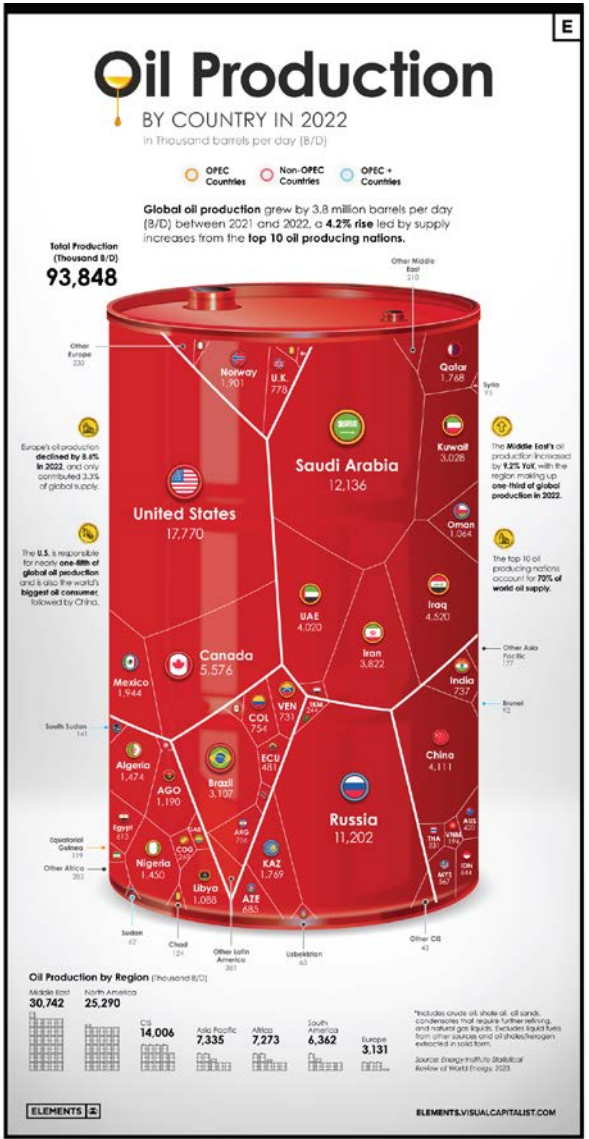
Petroleum Production by Country, 1980
World Total = 64 mmbd



Petroleum Production by Country, 2015
World Total = 96 mmbd

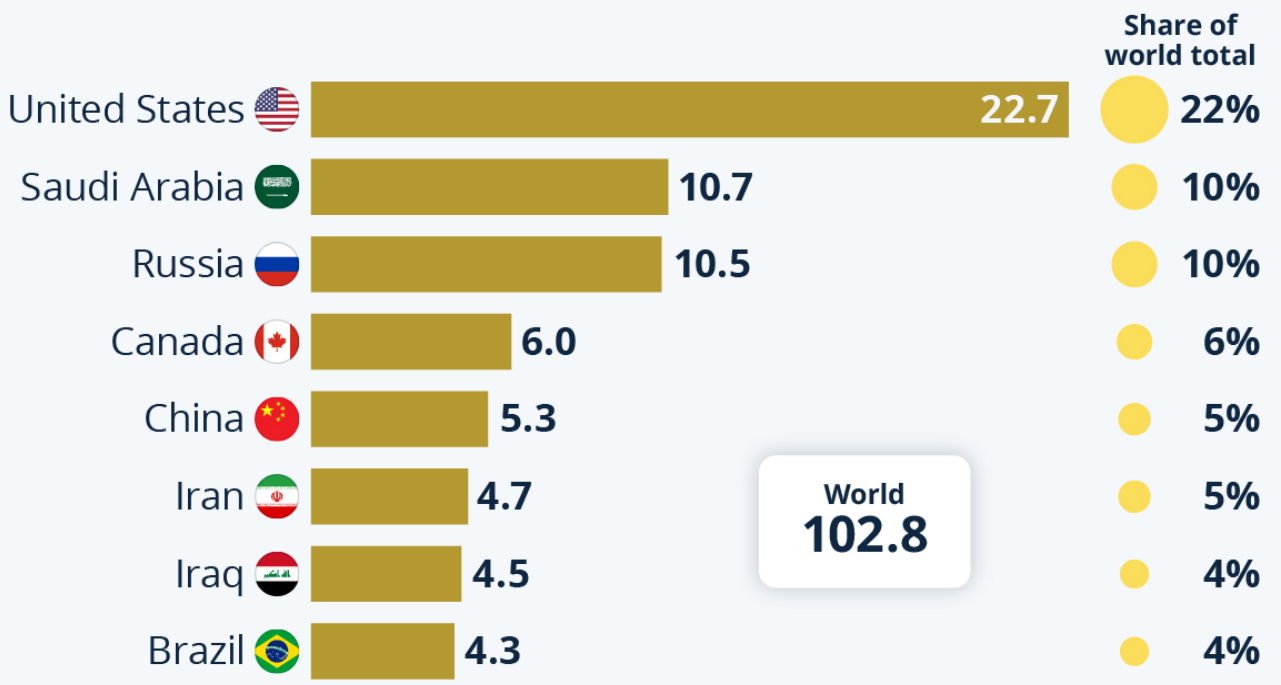


Major Petroleum Producing Countries



The World's Largest Oil Producers

Production of petroleum and other liquids in 2024 (in million barrels per day)*



* Includes crude oil (incl. lease condensate), natural gas plant liquids and other liquids
Source: U.S. Energy Information Administration

The Nature and Composition of Petroleum

❖ The Nature of Petroleum

- ❑ Petroleum is a naturally occurring, flammable, oily liquid found beneath the Earth's surface.
- ❑ It consists mainly of hydrocarbons but also contains small amounts of sulfur, nitrogen, and oxygen compounds.
- ❑ Physically, crude oil is usually brown to black in color, sometimes greenish, with a characteristic odor.
- ❑ It is less dense than water and insoluble in water, but soluble in organic solvents.
- ❑ Petroleum occurs in nature within porous sedimentary rocks, sealed by impermeable layers that trap it in reservoirs.

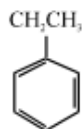
❖ Composition of Petroleum

Elemental Composition (approximate ranges):

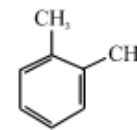
- **Carbon (C):** 83–87%
- **Hydrogen (H):** 11–15%
- **Sulfur (S):** 0.05–6%
- **Nitrogen (N):** 0.1–2%
- **Oxygen (O):** up to 1.5%



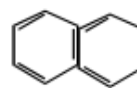
Benzene



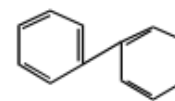
Ethylbenzene



1, 2-dimethylbenzene



Naphthalene



Biphenyl



The Nature and Composition of Petroleum

❖ Hydrocarbon Types:

❑ Paraffins (Alkanes):

- ❑ Straight- or branched-chain hydrocarbons (e.g., methane, hexane).
- ❑ Major component of petroleum.
- ❑ Important for fuels, but straight chains knock easily in engines, while branched chains give smoother combustion.

❑ Naphthenes (Cycloalkanes):

- ❑ Saturated ring compounds (e.g., cyclohexane).
- ❑ Contribute to fuel stability.

❑ Aromatics:

- ❑ Ring hydrocarbons with delocalized electrons (e.g., benzene, toluene, xylene).
- ❑ Higher energy content but also linked to health hazards.

❖ Non-Hydrocarbon Compounds:

❑ Sulfur compounds:

- H_2S , mercaptans, thiophenes (cause corrosion, pollution).

❑ Nitrogen compounds:

- pyridines, carbazoles (can poison refining catalysts).

❑ Oxygen compounds:

- phenols, naphthenic acids (affect acidity and stability).

❑ Trace metals:

- vanadium, nickel, etc., present in heavy crude.

PETROLEUM PROCESSING AND PRODUCTS

Table 1: Petroleum fractions

Boiling range (°C)	Composition (No. of carbon atoms per molecule)	Name	Main uses
<20	C ₁ to C ₄	Natural gas (gaseous compounds)	Fuel, chemical synthesis (i.e. raw material for chemical industry)
0-30	-	Natural gas (Zymogene and Rhigolene)	Liquid zymogene is used in the manufacture of ice. Rhigolene is used in medicine as local anaesthesia.
20-90	C ₅ to C ₇	Light petroleum (petroleum ether)	Solvent
30-150	C ₅ to C ₁₄	Crude naphtha	Solvent
70-90	C ₆ to C ₁₈	Gasoline of petrol	Motor fuel, solvent in dry cleaning
70-200	C ₆ to C ₁₀	Petrol (gasoline)	Motor fuel
90-120	C ₇ to C ₈	Ligroin (high b.p. petroleum ether or light petroleum)	Solvent in dry cleaning
100-200	C ₅ to C ₁₀	Fuel	Automobiles
120-160	C ₅ to C ₁₀	Benzene	Solvent (in dry cleaning and in oil and paint industry)
150-300	C ₁₀ to C ₃₈	Kerosine	Fuel, illuminant, making oil gas
175-300	C ₁₀ to C ₁₈	Kerosine (paraffin)	Fuel for jet engines or central heating systems
200-300	C ₁₂ to C ₁₈	Kerosine (paraffin)	Fuel (lamps and stoves)
>275	C ₁₂ to C ₂₀	Gas oil	Fuel for diesel engines
>300	C ₁₈ to C ₃₈	Gas oil or heavy oil	
300-400	C ₁₅ to C ₂₅	Diesel oil	Fuel (locomotive)
	C ₂₀ to C ₂₄	Lubricating oil	Lubricant (making candle, shoe polish, etc.)
>400	C ₂₁ to C ₃₀	Paraffin wax	Various
Non-volatile oil	> C ₂₀	Lubricating oils, waxes, etc.	Lubricant candles
Solid residue	> C ₄₀	Asphalt, bitumen	Road surfaces, roofing
		Vaseline	Lubricant
		Pitch	In toilet goods and ointment
		Petroleum coke (on redistillation of tar)	In paints and varnish. As fuel.

❖ Definition

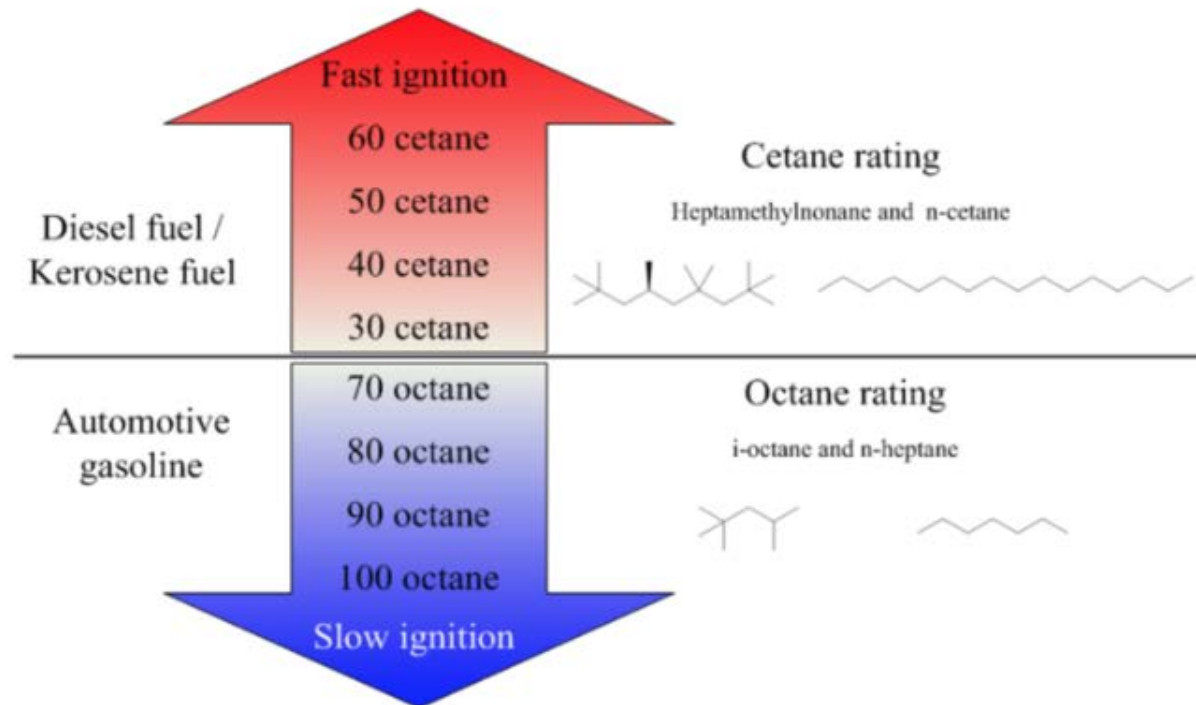
- ❑ The octane number (or octane rating) is a measure of a fuel's resistance to knocking (auto-ignition) in a spark-ignition engine.
- ❑ Knocking occurs when the air–fuel mixture in the cylinder ignites prematurely due to compression, causing a metallic "pinging" sound and engine damage.
- ❑ Fuels with higher octane numbers resist knocking better and allow for smoother engine operation.

Hydrocarbon	Motor method	Research method
Methane	110.0	107.5
Ethane	108.0	107.1
Propane	100.0	105.7
<i>n</i> -Butane	91.0	93.6
<i>n</i> -Pentane	61.7	61.7
<i>n</i> -Hexane	26.0	24.8
<i>n</i> -Heptane	0.0	0.0
<i>n</i> -Octane	−17.0*	−19.0*
Naphtha	41.0—56.0	43.0—58.0

Octane Number

❖ Reference Scale

Cetane and Octane Comparison



- ❑ The octane rating is defined by comparing the fuel to a mixture of two reference hydrocarbons:
 - **n-Heptane** → assigned an octane number of 0 (knocks very easily).
 - **Iso-octane (2,2,4-trimethylpentane)** → assigned an octane number of 100 (very resistant to knocking).
- ❑ **Example:** A gasoline with an octane number of 90 behaves the same, in terms of knocking tendency, as a mixture of 90% iso-octane and 10% n-heptane.

❖ Improvement of Octane Number

- ❑ In the past, the octane number was improved using tetraethyl lead (TEL) as an anti-knock additive.
- ❑ Due to environmental and health hazards, TEL has been phased out.
- ❑ Today, octane enhancement is achieved by:
 - Oxygenates such as ethanol and methanol.
 - Aromatic hydrocarbons (e.g., toluene, xylene).
 - Isomerization and reforming processes in refineries to produce branched hydrocarbons with higher octane.

❖ Significance

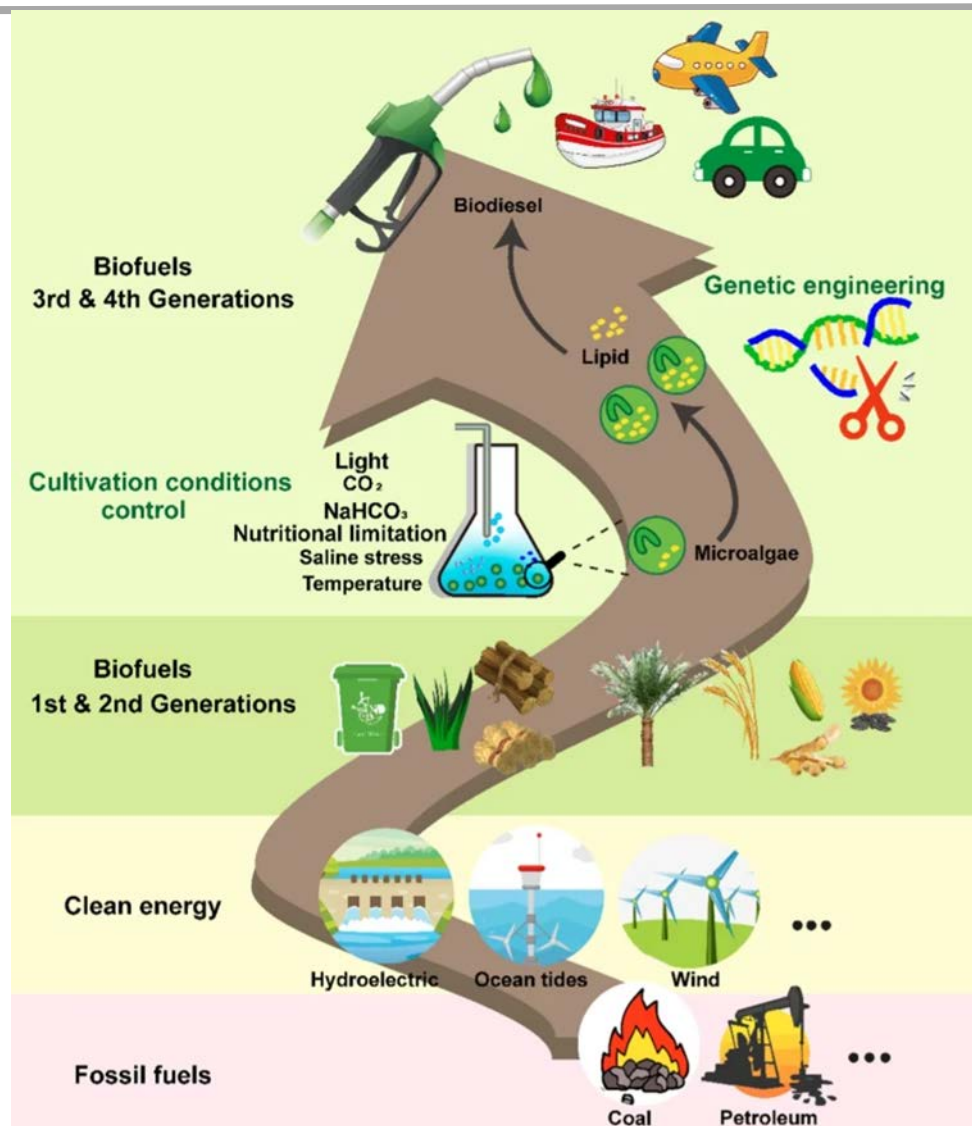
- ❑ A higher octane fuel allows:
 - Higher compression ratios in engines.
 - Greater efficiency and power output.
 - Reduced knocking and smoother performance.
- ❑ Common commercial gasoline grades:
 - Regular (≈ 87 octane)
 - Mid-grade (≈ 89 octane)
 - Premium (91–98 octane, depending on country).

USES OF PETROLEUM

❑ Petroleum has two main uses.

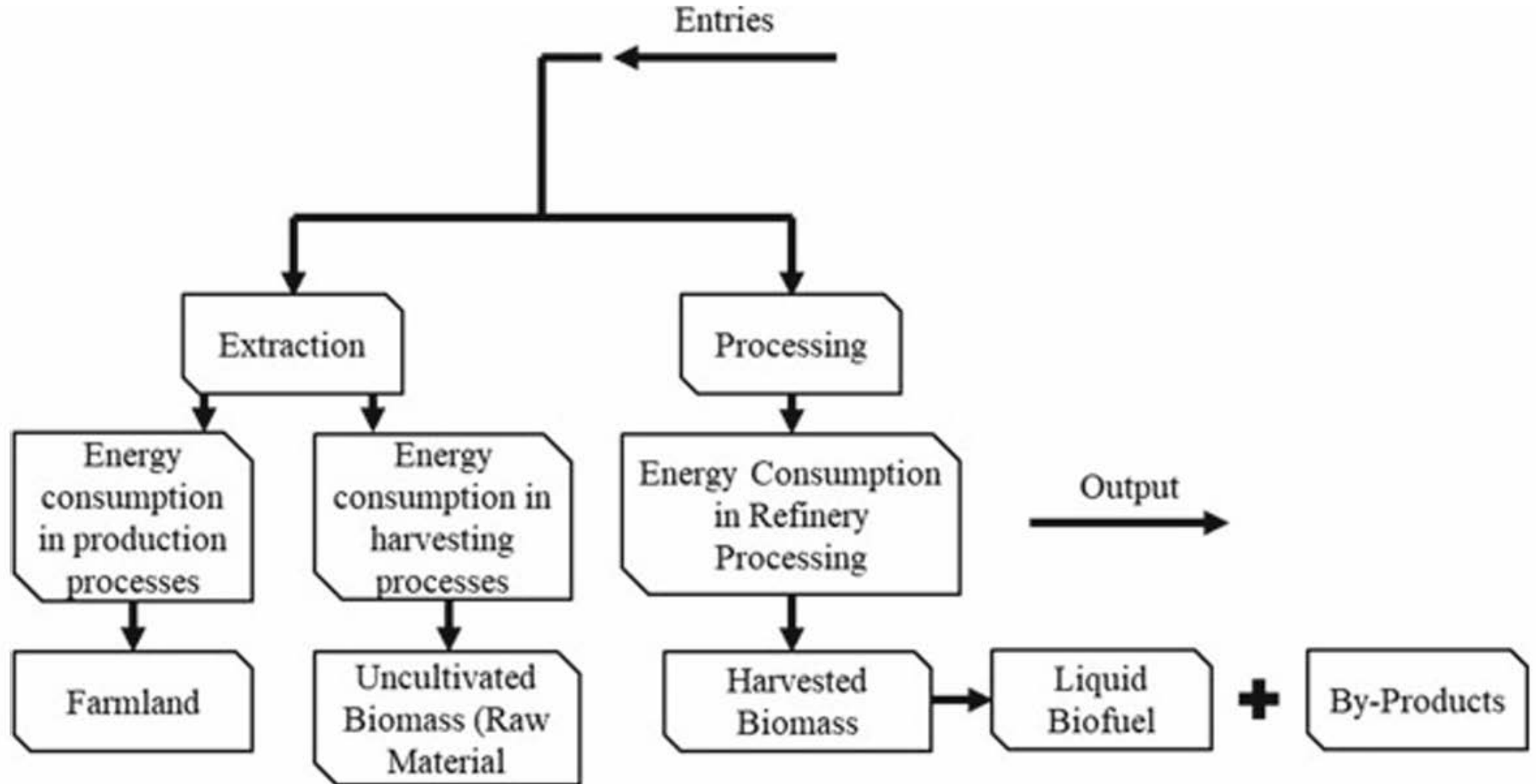
- The first is as a fuel The combustion of crude oil gave in-road to derivation of various energies from petroleum. Petroleum has been a source of energy for heating, lighting and locomotion and particularly the most convenient fuel for the internal combustion engine. This use has increased rapidly in importance with the coming of the motor car and a wide range of other applications of internal combustion engine (Bankole and Ogunkoya, 1978).
- The second use of petroleum is the synthesis of organic compounds. By 1965, about 80% of the world organic chemicals were synthesized from petroleum. This figure rose to 98% in 1980 and 99% in the year 2000. Thus, petroleum chemicals (petrochemicals) are a wide variety of chemicals. Commercially important ones include gasoline and kerosine. Petroleum jelly is a greasy gelatinous substance sourced from petroleum and used as ointment base, lubricant and protective covering (Arene and Kitwood, 1979).

Biofuels

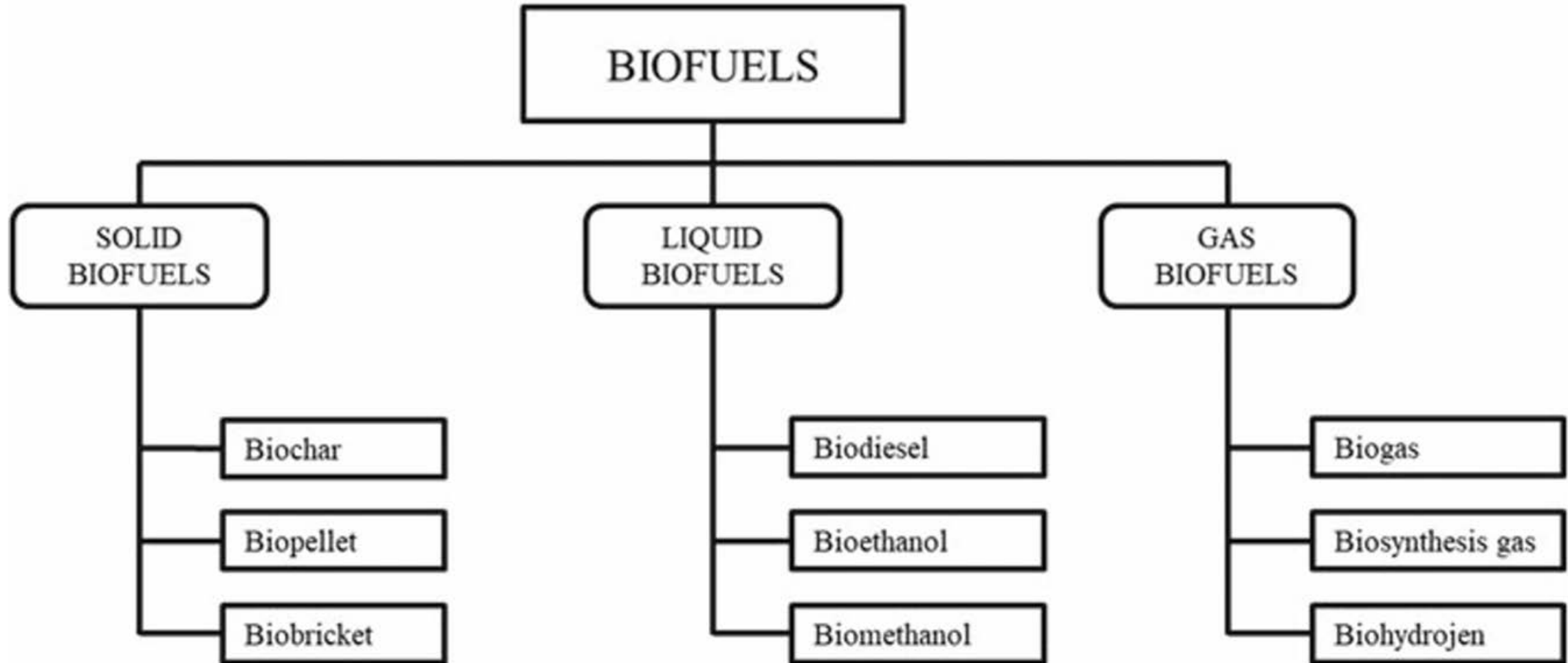


- The rapidly increasing world population, industrialization, and the environmental problems caused by the excessive use of fossil resources have gradually changed from a regional and national dimension to a global problem. Countries that do not want to be dependent on external energy and have problems in energy supply are trying to increase and diversify their alternative energy sources due to increasing environmental problems due to fossil resources. It can be said that alternative energy sources, which are unwanted in the past due to high costs, have become more attractive today due to technological developments. New and renewable energy sources are an important opportunity especially for countries that are dependent on foreign sources of energy.

Biofuel Production Processes



Classification of fuels of biological origin



Solid Biofuels



❑ Biofuels can be classified in different ways according to their sources and types. Biofuels that can be produced from forests, agricultural and fishery products or municipal wastes, agro-industry, food sector, and food sector products and wastes may be in the form of solid, ethanol, biodiesel, and pyrolysis fuels such as firewood, charcoal, and wood chips, or gas such as biogas. Biofuels:

- Primary (unprocessed)
- secondary (processed) biofuels.

Biofuels

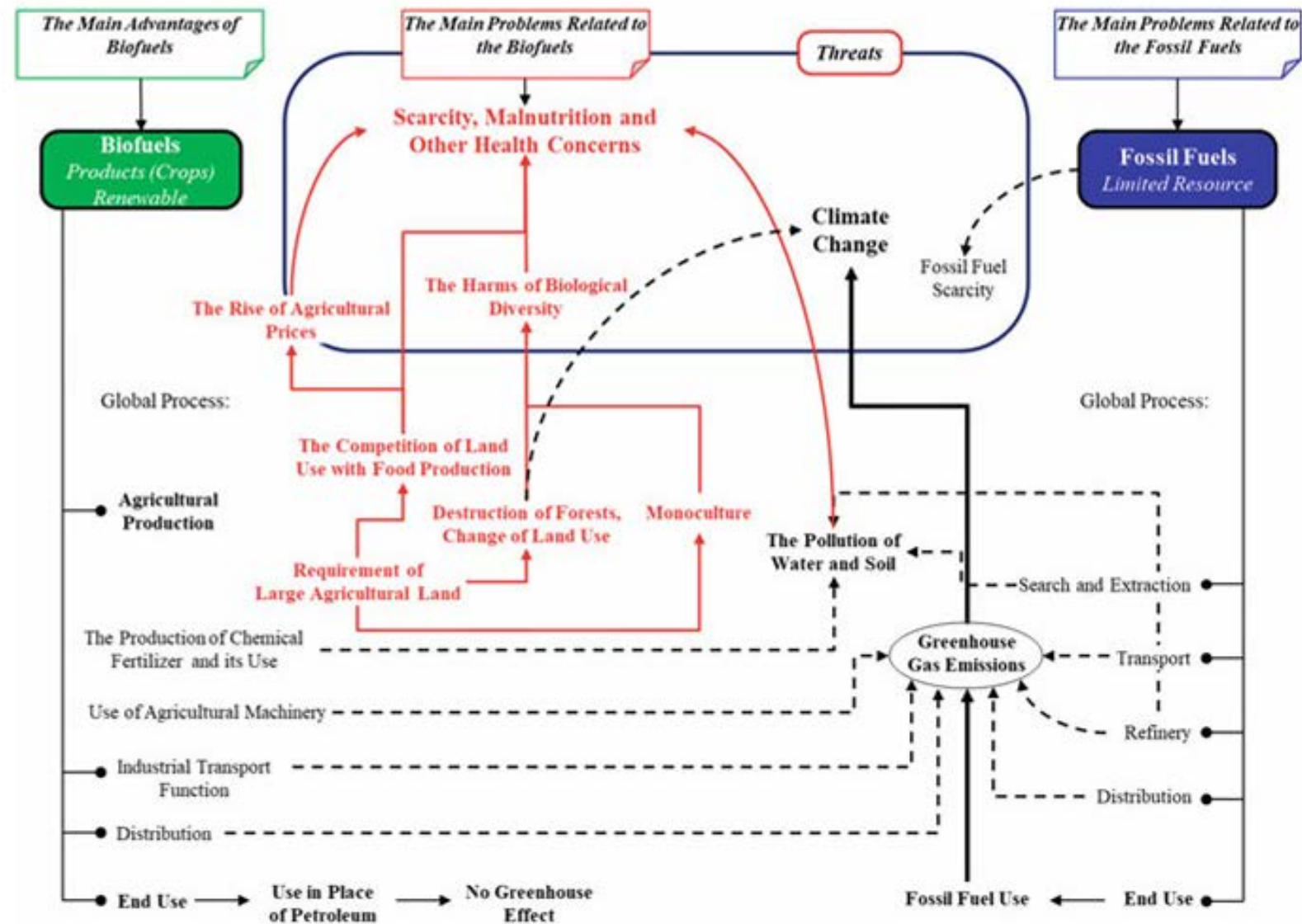
❑ **Primary biofuels:**

firewood, wood shavings, and parts thereof are organic materials used in their natural state. Burnt fuels are sources of energy that are often used for energy for cooking, heating, and energy production.

❑ **Secondary biofuels:**

solid (charcoal), liquid (ethanol, biodiesel, and other biofuels), and gases (biogas, synthetic gas, and hydrogen).

Main features of fossil and biofuel use



Productions of different generations Biofuel

