UNIT IV: SPECTROSCOPIC TECHNIQUES & NON CONVENTIONAL ENERGY SOURCES

Part A: SPECTROSCOPIC TECHNIQUES

Electromagnetic spectrum-UV (laws of absorption, instrumentation, theory of electronic spectroscopy, Frank-condon principle, chromophores and auxochromes, intensity shifts, applications), FT-IR (instrumentation and IR of some organic compounds, applications)-magnetic resonance imaging and CT scan (procedure & applications).

Part B: NON CONVENTIONAL ENERGY SOURCES

Design, working, schematic diagram, advantages and disadvantages of photovoltaic cell, hydropower, geothermal power, tidal and wave power, ocean thermal energy conversion.

Part A: SPECTROSCOPIC TECHNIQUES:-

Electromagnetic radition:-

- Electromagnetic radiation is a form of energy that is produced by oscillating electric and magnetic disturbance, or by the movement of electrically charged particles traveling through a vacuum or matter.
- The electric and magnetic fields come at right angles to each other and combined wave moves perpendicular to both magnetic and electric oscillating fields thus the disturbance.

General Properties of all electromagnetic radiation:

1. Electromagnetic radiation can travel through empty space. Most other types of waves must travel through some sort of substance. For example, sound waves need either a gas, solid, or liquid to pass through in order to be heard.
2. The speed of light is always a constant. (Speed of light : 2.99792458×10^8 m s^{-1})
3. Wavelengths are measured between the distances of either crests or troughs. It is usually characterized by the Greek symbol λλ.

Amplitude:-

- Amplitude is the distance from the maximum vertical displacement of the wave to the middle of the wave. This measures the magnitude of oscillation of a particular wave.

Wavelength

- Wavelength (λλ) is the distance of one full cycle of the oscillation. Longer wavelength waves such as radio waves carry low energy; this is why we can listen to the radio without any harmful consequences.

This wavelength frequently relationship is characterized by:

$$c=\lambda\nu$$

where

- c is the speed of light,

- λλ is wavelength, and
- νν is frequency.

Frequency

- Frequency is defined as the number of cycles per second, and is expressed as sec^{-1} or Hertz (Hz). Frequency is directly proportional to energy and can be express as: $E=h\nu$

where

E is energy,

h is Planck's constant, ($h= 6.62607 \times 10^{-34}$ J), and

ν is frequency.

➢ Electromagnetic spectrum:-

- Electromagnetic waves have an extremely wide range of wavelengths, frequencies, and energies.
- The highest energy form of electromagnetic waves are gamma (γ) rays and the lowest energy form are radio waves.

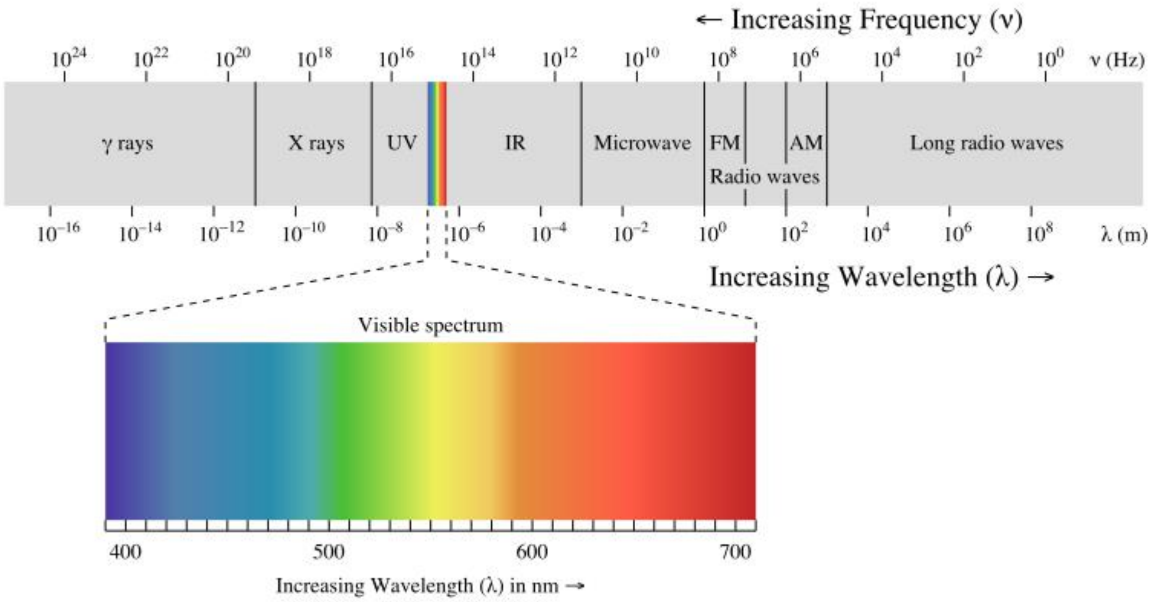


Fig:-Electromagnetic spectrum with light highlighted

- As a wave's wavelength increases, the frequency decreases, and as wave's wavelength decreases, the frequency increases.
- When electromagnetic energy is released as the energy level increases, the wavelength decreases and frequency decreases.
- Thus, electromagnetic radiation is then grouped into categories based on its wavelength or frequency into the electromagnetic spectrum.

- The different types of electromagnetic radiation shown in the electromagnetic spectrum consists of radio waves, microwaves, infrared waves, visible light, ultraviolet radiation, X-rays, and gamma rays. The part of the electromagnetic spectrum that we are able to see is the visible light spectrum.

- **laws of absorption:-**

- Absorption of light takes place when matter captures electromagnetic radiation, converting the energy of photons to internal energy.
- Energy is transferred from the radiation to the absorbing species**.**

The Effect of Light Absorption on Matter:-

- Since the energy levels of matter are quantized, only light of energy that can cause transitions from one existing energy level to another will be absorbed.
- We describe the energy change in the absorber as a transition or an excitation from a lower energy level to a higher energy level.

- **Instrumentation and working of the UV spectrometers:-**

Instrumentation and working of the UV spectrometers can be studied simultaneously. Most of the modern UV spectrometers consist of the following parts-

- **Light Source**- Tungsten filament lamps and Hydrogen-Deuterium lamps are most widely used and suitable light source as they cover the whole UV region.

- **Amplifier**- The alternating current generated in the photocells is transferred to the amplifier. The amplifier is coupled to a small servometer.

- **Recording devices**- Most of the time amplifier is coupled to a pen recorder which is connected to the computer. Computer stores all the data generated and produces the spectrum of the desired compound.

- **Photometer:-**
  An instrument for measuring the intensity of light or the relative intensity of a pair of lights.Also called an illuminometer. It utilizes filter to isolate a narrow wavelength region**.**

- **Spectrophotometer:-**
  An instrument measures the ratio, or a function of the two, of the radiant power of two EM beams over a large wavelength region.

- **Colorimeter:-**
  An instrument which is used for measuring absorption in the visible region is generally called colorimeter.

- **Theory of electronic spectroscopy:-**

- **Electron spectroscopy** is an analytical technique to study the electronic structure and its dynamics in atoms and molecules.
- In general an excitation source such as x-rays, electrons or synchrotron radiation will eject an electron from an inner-shell orbital of an atom.
- Detecting photoelectrons that are ejected by x-rays is called x-ray photoelectron spectroscopy(XPS) or electron spectroscopy for chemical analysis (ESCA).
- Detecting electrons that are ejected from higher orbitals to conserve energy during electron transitions is called Auger electron spectroscopy (AES).
- Experimental applications include high-resolution measurements on the intensity and angular distributions of emitted electrons as well as on the total and partial ion yields.

Various methods emanate from the electron spectroscopy are:

- Electron spectroscopy for chemical Analysis
- Auger electron spectroscopy

Electron spectroscopy for chemical Analysis:-

In typical laboratory use, a sample is placed in the specimen chamber of a scanning electron microscope (SEM). Because the SEM uses a beam of electrons to illuminate the sample and produce the three dimensional images often seen in lay news reports and publications as well as professional journals, the sample must be able to conduct electricity

Auger electron spectroscopy (**AES**) is a common analytical technique used specifically in the study of surfaces and, more generally, in the area of materials science.

- **Frank-condon principle**:-
  - The Franck–Condon principle is a rule in spectroscopy and quantum chemistry that explains the intensity of vibronic transitions.
  - Vibronic transitions are the simultaneous changes in electronic and vibrational energy levels of a molecule due to the absorption or emission of a photon of the appropriate energy.
  - It states that when a molecule is undergoing an electronic transition, such as ionization, the nuclear configuration of the molecule experiences no significant change.
  - This is due in fact that nuclei are much more massive than electrons and the electronic transition takes place faster than the nuclei can respond.
  - When the nucleus realigns itself with the new electronic configuration, the theory states that it must undergo a vibration.

- **CHROMOPHORE:**

- The term chromophore was previously used to denote a functional group of some other structural feature of which gives a color to compound.
- For example- Nitro group is a chromophore because its presence in a compound gives yellow color to the compound.
- But these days the term chromophore is used in a much broader sense which may be defined as "any group which exhibit absorption of electromagnetic radiation in a visible or ultra-visible region "It may or may not impart any color to the compound.
- Some of the important chromophores are: ethylene, acetylene, carbonyls, acids, esters and nitrile groups etc.

AUXOCHROMES:

- It is a group which itself does not act as a chromophore but when attached to a chromophore, it shifts the adsorption towards longer wavelength along with an increase in the intensity of absorption.
- Some commonly known auxochromic groups are: -OH, $-NH_2$, -OR, -NHR, and $–NR_2$.

intensity shifts:-

There are four types of shifts observed in the UV spectroscopy-

a) **Bathochromic effect:**-
This type of shift is also known as red shift.
Bathochromic shift is an effect by virtue of which the absorption maximum is shifted towards the longer wavelength due to the presence of an auxochrome or change in solvents.

b) **Hypsochromic shift-** This effect is also known as blue shift. Hypsochromic shift is an effect by virtue of which absorption maximum is shifted towards the shorter wavelength. Generally it is caused due to the removal of conjugation or by changing the polarity of the solvents.

c) **Hyperchromic effect** - Hyperchromic shift is an effect by virtue of which absorption maximum increases. The introduction of an auxochrome in the compound generally results in the hyperchromic effect.

d) **Hypochromic effect**- Hyperchromic effect is defined as the effect by virtue of intensity of absorption maximum decreases. Hyperchromic effect occurs due to the distortion of the geometry of the molecule with an introduction of new group.

Applications of UV spectroscopy:-

1. **Detection of functional groups-** UV spectroscopy is used to detect the presence or absence of chromophore in the compound.

This is technique is not useful for the detection of chromophore in complex compounds.
The absence of a band at a particular band can be seen as an evidence for the absence of a particular group.

2. **Detection of extent of conjugation**- The extent of conjugation in the polyenes can be detected with the help of UV spectroscopy. With the increase in double bonds the absorption shifts towards the longer wavelength.
3. **Identification of an unknown compound**- An unknown compound can be identified with the help of UV spectroscopy. The spectrum of unknown compound is compared with the spectrum of a reference compound and if both the spectrums coincide then it confirms the identification of the unknown substance.
4. .**Determination of configurations of geometrical isomers**- It is observed that cis-alkenes absorb at different wavelength than the trans-alkenes. The two isomers can be distinguished with each other when one of the isomers has non-coplanar structure due to steric hindrances.

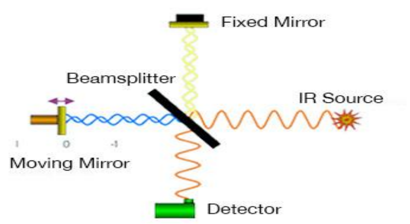
➢ FT-IR:-

- FTIR stands for Fourier transform infrared, the preferred method of infrared spectroscopy.
- When IR radiation is passed through a sample, some radiation is absorbed by the sample and some passes through (is transmitted).
- The resulting signal at the detector is a spectrum representing a molecular ‘fingerprint’ of the sample.
- The usefulness of infrared spectroscopy arises because different chemical structures (molecules) produce different spectral fingerprints.

So, what is FTIR?

- The Fourier Transform converts the detector output to an interpretable spectrum.
- The FTIR generates spectra with patterns that provide structural insights.

How does FTIR work and why use it?



The FTIR uses interferometry to record information about a material placed in the IR beam. The Fourier Transform results in spectra that analysts can use to identify or quantify the material.

- An FTIR spectrum arises from interferograms being 'decoded' into recognizable spectra
- Patterns in spectra help identify the sample, since molecules exhibit specific IR fingerprints.

➢ **IR of some organic compounds**:-

- IR (infrared) spectroscopy is useful in organic chemistry because it enables you to identify different functional groups.
- This is because each functional group contains certain bonds, and these bonds always show up in the same places in the IR spectrum.
- To generate the IR spectrum, different frequencies of infrared light are passed through a sample, and the transmittance of light at each frequency is measured.
- Different functional groups produce bond absorptions at different locations and intensities on the IR spectrum.
- This table lists the locations and intensities of absorptions produced by typical functional groups.

IR Absorptions of Common Functional Groups

Functional Group	*Absorption Location (cm^{-1})*	*Absorption Intensity*
Alkane (C–H)	2,850–2,975	Medium to strong
Alcohol (O–H)	3,400–3,700	Strong, broad
Alkene (C=C) (C=C–H)	1,640–1,680 3,020–3,100	Weak to medium Medium
Alkyne (C≡C) (C≡C–H)	 2,100–2,250 3,300	 Medium Strong
Nitrile (C≡N)	2,200–2,250	Medium
Aromatics	1,650–2,000	Weak
Amines (N–H)	3,300–3,350	Medium
Carbonyls (C=O) Aldehyde (CHO) Ketone (RCOR) Ester (RCOOR) Acid (RCOOH)	 1,720–1,740 1,715 1,735–1,750 1,700–1,725	Strong

➢ **Sampling and applications of FTIR:-**

- FTIR can be a single purpose tool or a highly flexible research instrument. With the FTIR configured to use a specific sampling device – transmission or ATR for instance – the spectrometer can provide a wide range of information:

- Most commonly, the identification of an unknown
- Quantitative information, such as additives or contaminants
- Kinetic information through the growth or decay of infrared absorptions
- Or more complex information when coupled with other devices such as TGA, GC or Rheometry

Ultimately, FTIR can be a cost-effective answer machine.

➢ Magnetic resonance:-

- Magnetic Resonance (MR) spectroscopy is a noninvasive diagnostic test for measuring biochemical changes in the brain, especially the presence of tumors.
- While magnetic resonance imaging (MRI) identifies the anatomical location of a tumor, MR spectroscopy compares the chemical composition of normal brain tissue with abnormal tumor tissue.

How does MR spectroscopy work?

- MR spectroscopy is conducted on the same machine as conventional MRI. The MRI scan uses a powerful magnet, radio waves, and a computer to create detailed images.
- MR spectroscopy analyzes molecules such as hydrogen ions or protons.
- Proton spectroscopy is more commonly used.
- There are several different metabolites, or products of metabolism, that can be measured to differentiate between tumor types:
  - Amino acids
  - Lipid
  - Lactate
  - Alanine
  - N-acetyl aspartate
  - Choline
  - Creatine
  - Myoinositol

➢ Magnetic Resonance Imaging (MRI) & CT scan

- MRI is a non-invasive imaging technology that produces three dimensional detailed anatomical images.
- It is often used for disease detection, diagnosis, and treatment monitoring.
- It is based on sophisticated technology that excites and detects the change in the direction of the rotational axis of protons found in the water that makes up living tissues

How does MRI work?

- MRIs employ powerful magnets which produce a strong magnetic field that forces protons in the body to align with that field.
- When a radiofrequency current is then pulsed through the patient, the protons are stimulated, and spin out of equilibrium, straining against the pull of the magnetic field.
- To obtain an MRI image, a patient is placed inside a large magnet and must remain very still during the imaging process in order not to blur the image.

What is MRI used for?

- MRI scanners are particularly well suited to image the non-bony parts or soft tissues of the body.

- They differ from computed tomography (CT), in that they do not use the damaging ionizing radiation of x-rays.
- The brain, spinal cord and nerves, as well as muscles, ligaments, and tendons are seen much more clearly with MRI than with regular x-rays and CT; for this reason MRI is often used to image knee and shoulder injuries.
- In the brain, MRI can differentiate between white matter and grey matter and can also be used to diagnose aneurysms and tumors.
- Because MRI does not use x-rays or other radiation, it is the imaging modality of choice when frequent imaging is required for diagnosis or therapy, especially in the brain.
- However, MRI is more expensive than x-ray imaging or CT scanning.
- One kind of specialized MRI is functional Magnetic Resonance Imaging (fMRI.)
- This is used to observe brain structures and determine which areas of the brain “activate” (consume more oxygen) during various cognitive tasks.
- It is used to advance the understanding of brain organization and offers a potential new standard for assessing neurological status and neurosurgical risk.

Non-conventional Energy sources :— Introduction.

→ Non-conventional energy are those sources which are renewable and ecologically safe. such as solar energy, wind energy, ocean energy, geothermal energy, neuclear energy etc.

→ The importance of using non-conventional or renewable power was recognized by in India early 1970.

1. Solar energy: It is utilized in India through photovolatanic route and thermal route

2. Biomass: Power based on biomass were launched in different placed in central India.

3. Wind Energy: wind energy is used for power generation.

4. Geothermal Energy: Geothermal energy generated from hot springs. It is generated in Himachal pradesh and Jammu & kashmir.

5. Energy from urban and industrial waste :—

→ Power is generated from urban waste, which is in practise in Timarpur in Delhi and Tamil Nadu.

⇒ SOLAR ENERGY :—

Introduction :—

→ solar energy is a renewable & ecofriendly energy.

→ The energy received by the earth in the form of electro-magnetic radiation is known as solar energy.

→ The solar energy is cheap and pollution free.

→ The solar energy is used to generate electricity by using solar cells.

→ Solar cell is a form of photovoltaic cell.

solar cell : A solar cell is an electrical device that converts the energy of light directly into electricity by photovoltaic cell.

Photovoltaic cell :

→ The term photovoltaic comes from greek word "Phos" meaning light and volt is the unit of emf. which was named by inventer of the battery the italian physicist Alessandro volta.

→ This term photo-voltaic is used in since 1849.

→ specially, it is used to generate electricity from sun light, lamp light or artificial light.

~~Working of photovoltaic cells~~ : —

Principle :

→ Solar cells employ (use) the principle of 'Photovoltaic effect' for energy conversion.

→ A material generate electricity when exposed directly to sun light. This is also known as photovoltaic effect

Construction :

→ Solar cells employ two semi-conductors namely p-type semiconductor and n-type semiconductor.

→ p-type semiconductor is usually a silicon doped with Boron impurities.

→ n-type semiconductor is a silicon doped with either Phosphorous or arsenic.

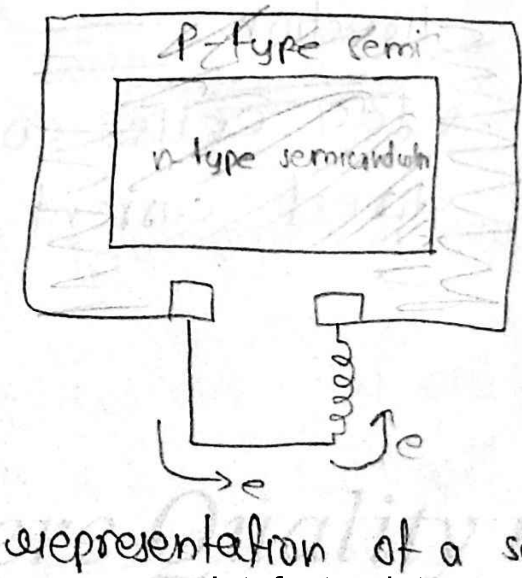
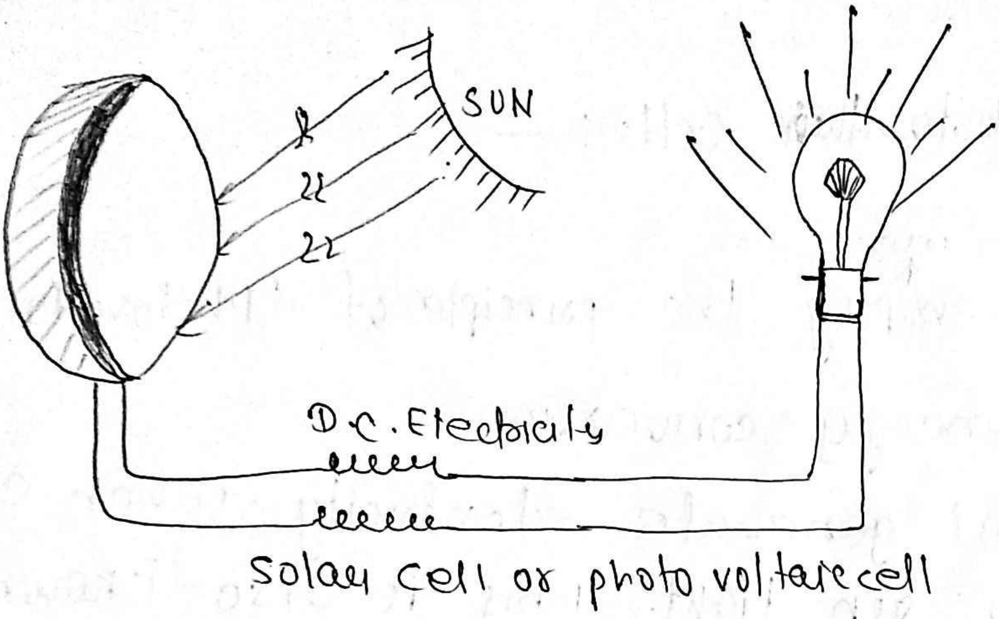


Fig:(1) representation of a solar cells.



Fig(2): schematic Diagram of a Solar cell.

* A solar photovoltaic cell works on the following steps:—

1. Photon in sunlight hits the panel and absorbed, by semi conducting material such as silicon.

2. The electrons present in the material are delocalised allowing to flow through the material to produce electricity. Due to special composition of solar cells the electrons are allow to move in single direction

3. An array of solar cells converts solar energy into the direct current which can be used.

1600
300
3000

Applications of solar energy:—

1. Solar water heating
2. Heating and cooling of residential building
3. Solar cookers
4. Solar engines for water pumping
5. Power generation by solar ponds.
6. Solar photo voltaic cell etc

⇒ Non-conventional Energy sources:—

Hydero power:—

→ Flowing water creates energy that can be captured and turned into electricity.

→ The power available depend on the rate at which the water is flowing and the height which it falls down

The hydero schemes are classified into four types:—

1. Large scale: where power output is about 2 MW and above
2. Mini scale: where the output power is 100 KW – 200 KW
3. Micro scale: 5 KW – 100 KW
4. Pico scale: less than 5 KW.

→ The core of hydro scheme is the turbine, which is rotated by moving water.

→ Different types of turbines are used depending on the head and flow of the site.

- Pelton turbines are used for low flow of water
- Francis turbines are used for high flow and cross flow of water
- Propeller turbines are used for large flow of water.

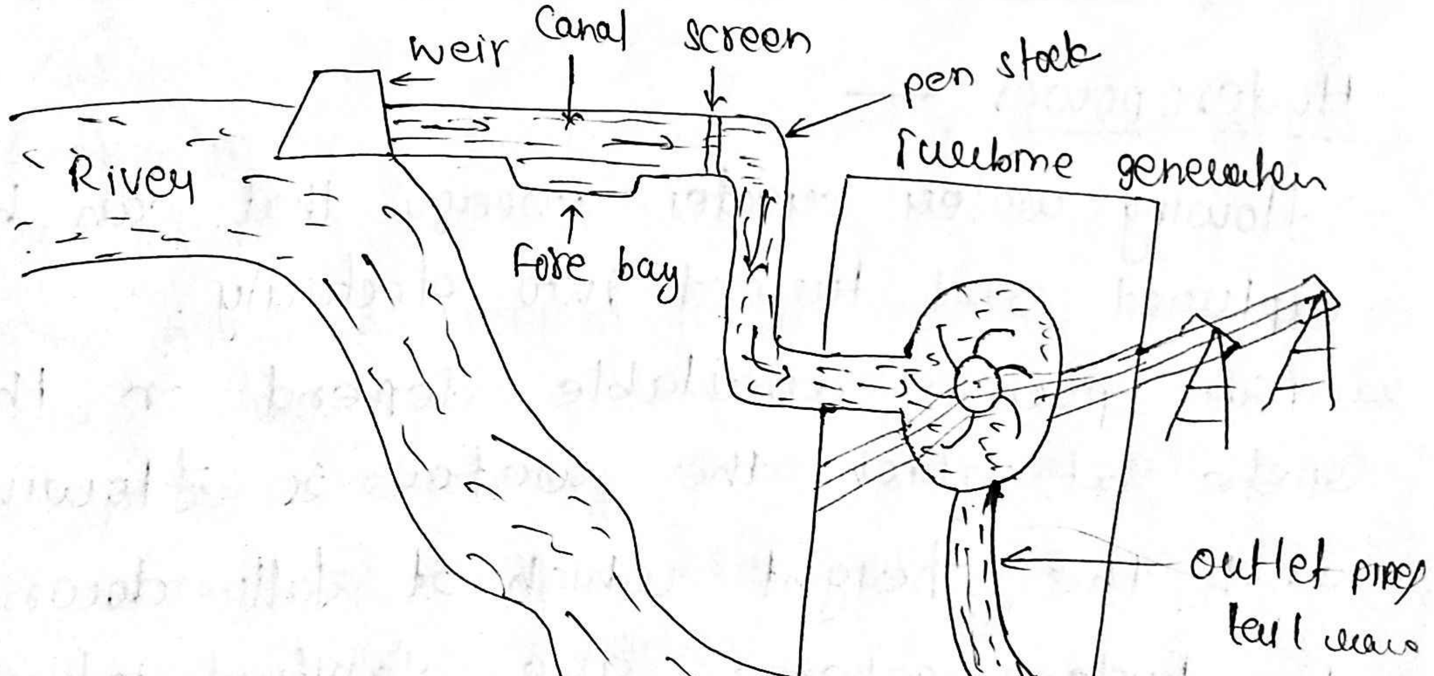


fig: Generation of hydro power

→ A small dam in the river bed directs the water to a settling tank (weir).

-> The water and clean water flow in to a canal.
-> A pipe to settling tank called forebay.
-> water flows out into a pipe called penstock.

Geothermal Energy:-

-> Geothermal energy is the heat from the earth.
-> Resources of geothermal energy range from shallow ground to hot water and hot rock.
-> The first geothermal electricity was produced in Italy in 1904.
-> To produce geothermal ~~energy~~ electricity, wells sometimes 1.6 kms deep or more drilled into the underground reservoirs and very hot water that drives turbines and turbines drive electricity generators.

Three types of geothermal power plants :-

1. Dry steam.
2. Flash
3. Binary

1. Dry steam geothermal generator takes steam out of fractures in the ground and uses it directly to drive turbines.

2. Flash geothermal plants pull deep, high pressure hot water into cooler, low pressure water

3. Binary geothermal plants, the hot water is passed by a secondary fluid, with much lower boiling point than water, producing vapour of the secondary fluid, which can drive turbine

→ Most geothermal plant in future will be binary plants

→ Geothermal plants have advantages over other thermal plants, that no fossil fuel is burned, no emmision of CO_2 and other gases and conversion

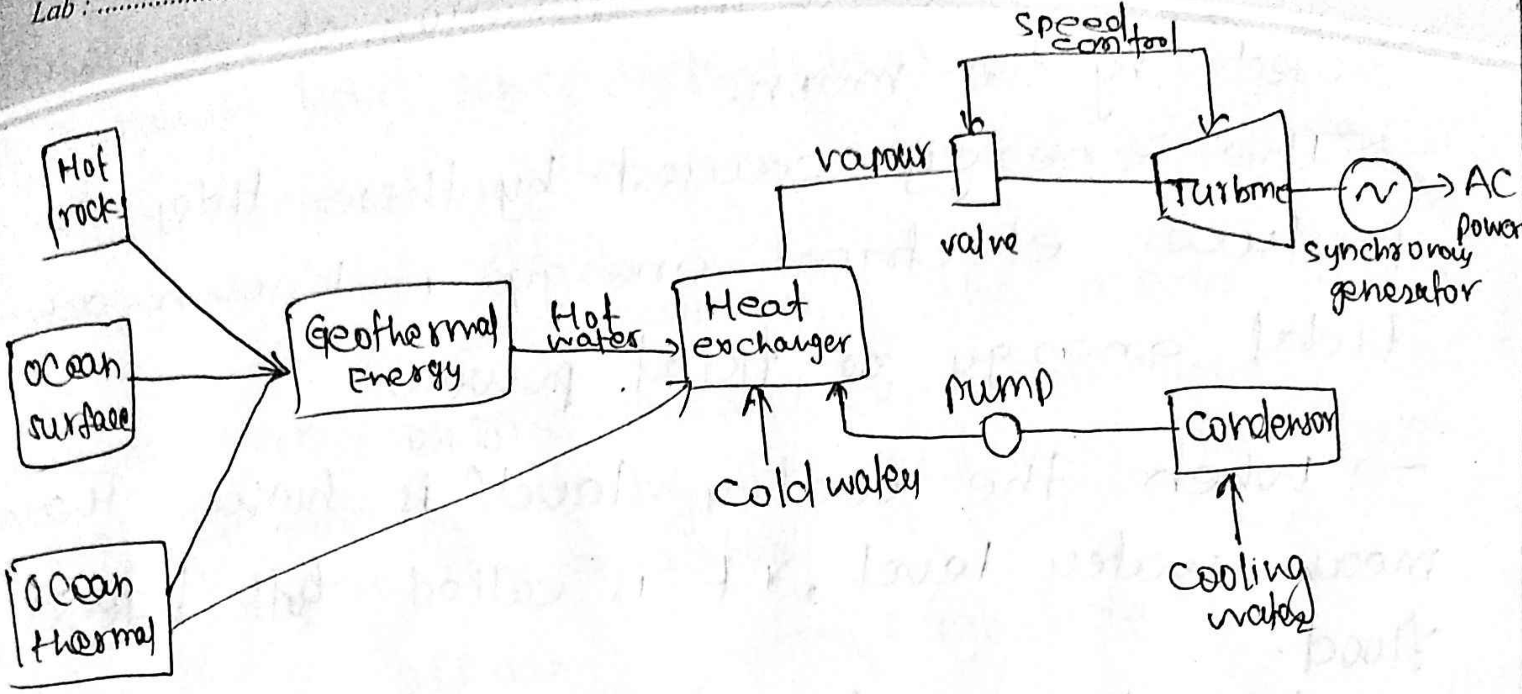


fig: geothermal power generator (Binary system)

Tidal and wave Power :

→ Tidal power is also called tidal energy.

→ It is a form of hydro power that converts the energy obtained from tides into electricity.

→ Tidal energy have potential for future electricity generation

→ Tides are more predictable than wind energy and solar power, but tidal energy is more costly and limited availability of sites.

→ The world largest tidal power plant in france.

→ Tidal is a periodic rise and fall of water level of sea due to the attraction of sea water caused by the moon.

→ The energy caused by these tides to produce electrical energy is known as tidal energy or tidal power.

→ When the water level of sea is higher than mean water level, it is called full tide or flood.

→ when the water level is below the mean water level of sea. it is called as Ebb tide

Tidal power is generated in four methods:

1. Tidal steam generator (TSG):

→ This method make use of the kinetic energy of moving water to power turbines in a similar way as wind power turbines.

→ These turbines can be horizontal, vertical, open or ducted and placed near the bottom of the water column.

2. Tidal barrage method:

→ Tidal barage make use of the potential energy difference of high and low tides.

3. Dynamic tidal power method (DTP):—

→ The interaction between potential and kinetic energy in tidal flows.

→ Long dams are built into the ocean without enclosing an area, leading to a significance water level difference producing low and high tides from which power is generated.

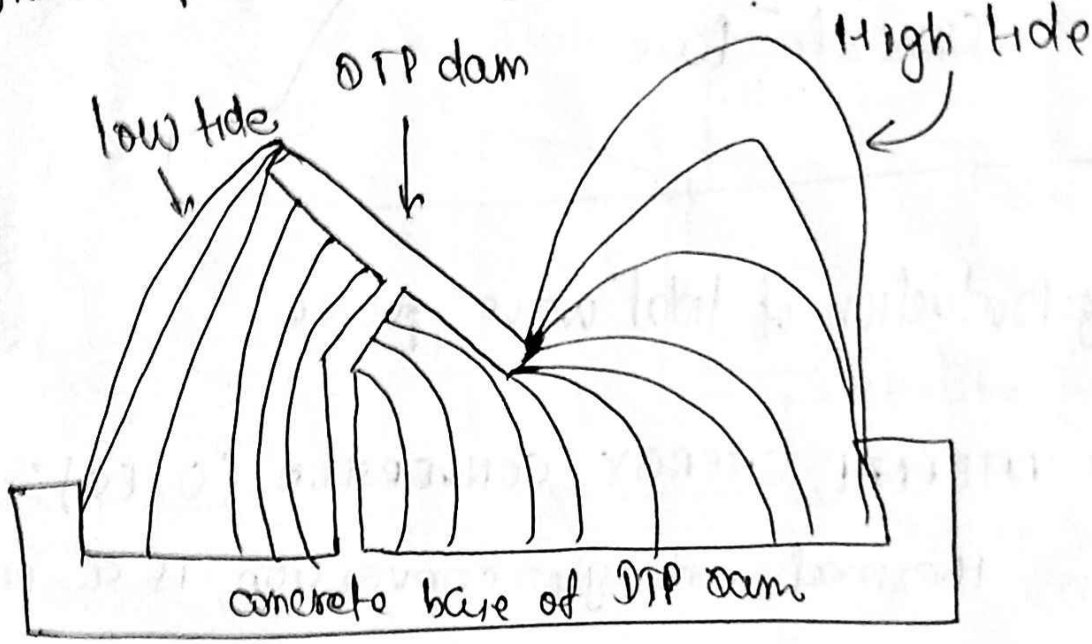


fig. Top down view of a DTP dam

4. <u>Tidal lagoon</u>:

→ A newer tidal energy design is to construct circular retaining walls embeded with turbines that can capture the potential energy of tides.

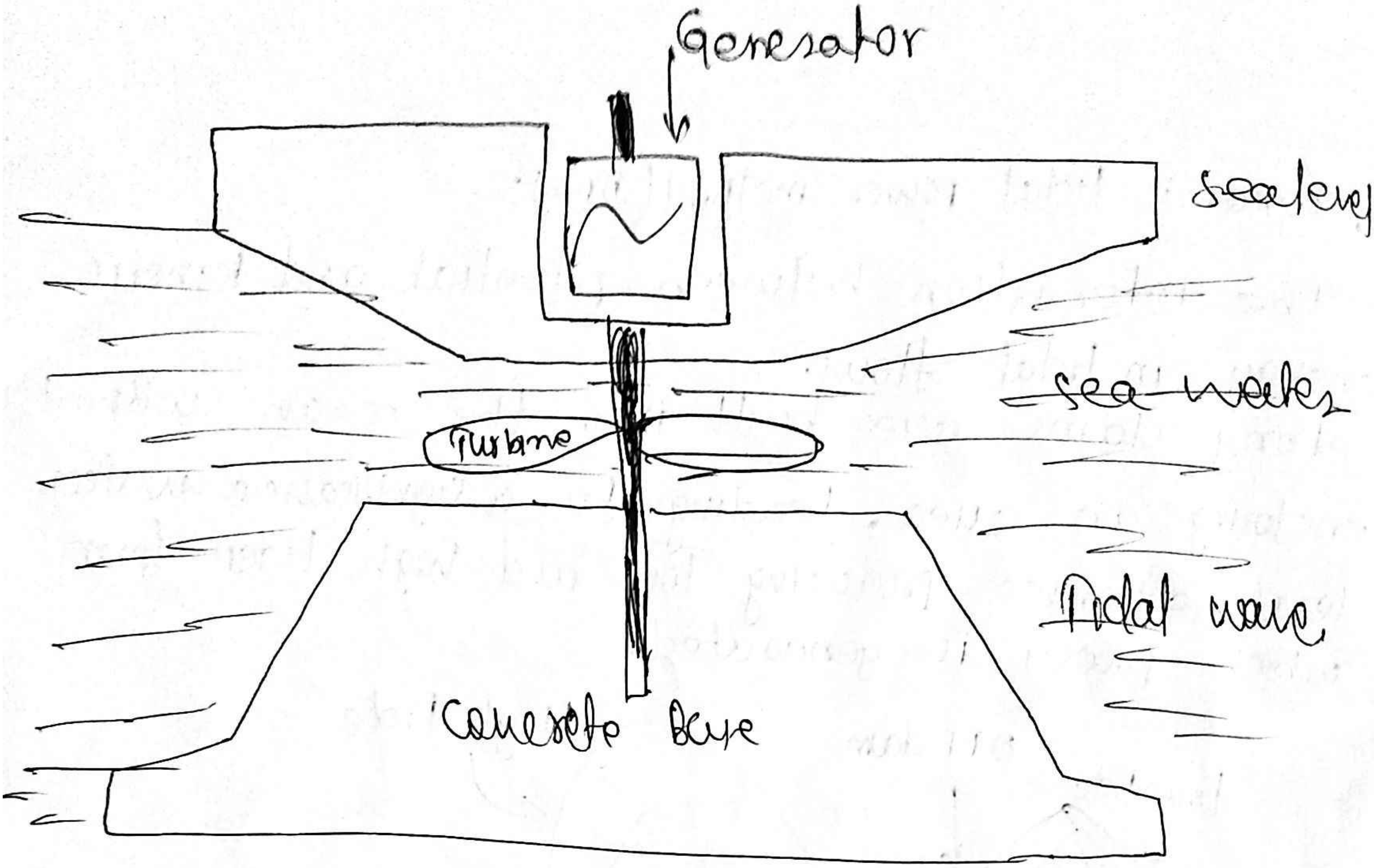


Fig: Production of tidal wave power

OCEAN THERMAL ENERGY CONVERSION (OTEC):-

→ ocean thermal energy conversion is a process that can produce electricity by using the temperature difference between cold ocean water and warm tropical surface water.

→ OTEC is base loaded electricity generation

→ OTEC theory was devloped in 1880 and constructed in 1926.

Three Types of OTEC:

1. closed cycle systems:

→ These systems use fluid with a low boiling point such as ammonia (B.P = -33°C) to power a turbine to generate electricity.

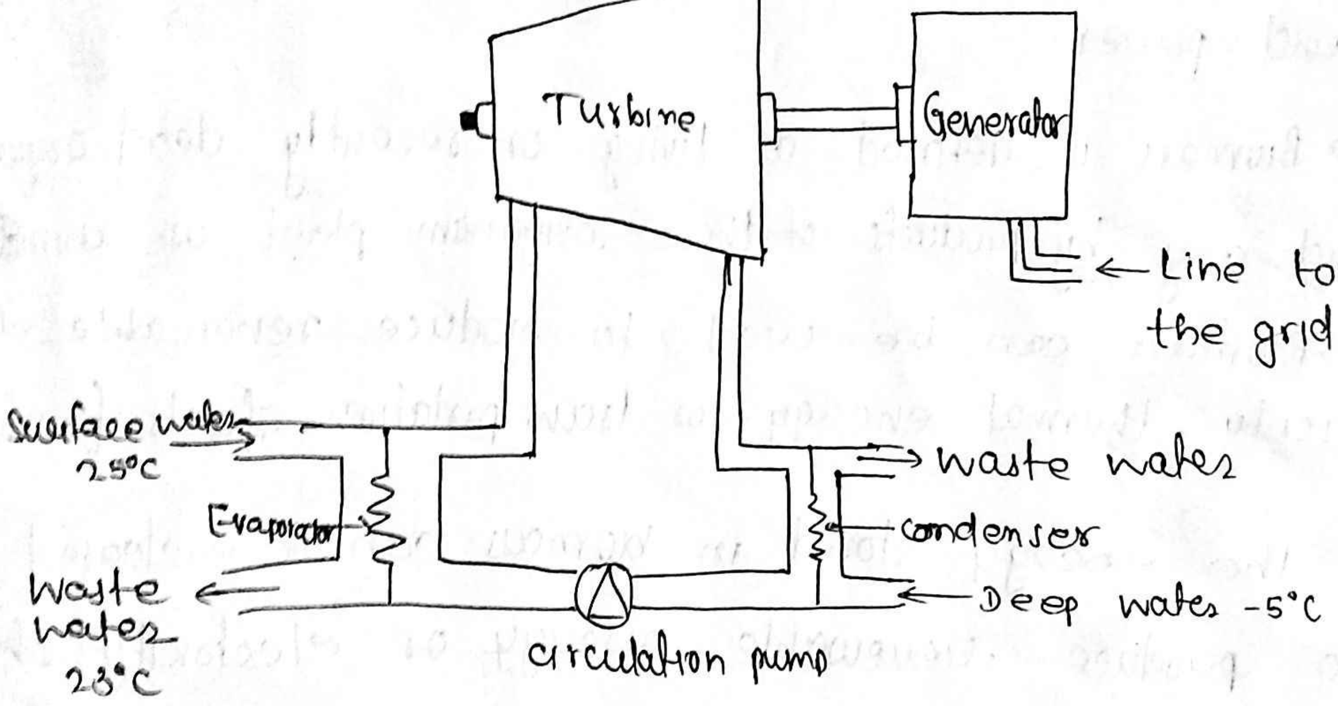


Fig: closed cycle OTEC plant.

2. Open cycle OTEC:

→ open cycle OTEC uses warm surface water directly to make electricity

3. Hybrid OTEC:

→ A hybrid cycle combines the features of closed and open cycle systems.

BIOMASS & BIOFUELS.

→ The term biomass refers to organic matter such timber and crops to be burnt to generate heat and power.

→ Biomass is defined as living or recently dead organisms and any by-products of those organism plant or animal.

→ Biomass can be used to produce renewable electricity, thermal energy or transportation fuels (bio fuels)

→ The energy stored in biomass can be released to produce renewable ~~energy or~~ electricity or heat

The most common biomass feed stocks are:

1. Grains and starch crops like suger cane, iron, wheat, sugar beets and instrial sweet potatoes.
2. Food waste
3. Forestry materials
4. Animal by-products
5. Energy crops.