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From Editor's desk

It is a proud privilege on our behalf to announce the publication of July 2020 issue of CHEMEDGE, the half yearly Students' technical magazine of the Department of Chemical Engineering, Heritage Institute of Technology, Kolkata. The aim of this technical magazine is to encourage students of Chemical Engineering Department to contribute articles on novel and interesting topics related to recent technical development and new innovations in the fields of chemical engineering and allied disciplines. Students have prepared their technical write up based on various published research articles, newsletter and other open access academic materials as resources.

In the present issue, topics on various challenges such as bioremediation of oil spill, radioactive waste management, production of biodiesel from waste plastics, carbon dioxide capture using metal organic framework have been covered and compiled. Students have also compiled various innovative ideas including drug formulation and discovery, nanosensor and its application, production of biodegradable plastics from organic waste in this issue.

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DNA Based Nanobiosensors for the Detection of Diseases

Detection of disease at an early stage is one of the biggest challenges in medicine. Different disciplines of science are working together in this regard. Nanotechnology is having a profound impact on the development of a new class of biosensors known as nanobiosensors. Nanobiosensors commonly comprise a biological recognition molecule immobilized onto the surface of a signal transducer. The reaction between the bio-recognition molecule and the analyte is a heterogeneous reaction and therefore the design of the biosensing interface is important in determining the performance of the nanobiosensor. The goal of nanodiagnostics is to provide more accurate tools for earlier diagnosis, to reduce cost and to simplify healthcare delivery of effective and personalized medicine, especially with regard to chronic diseases that have high healthcare cost.

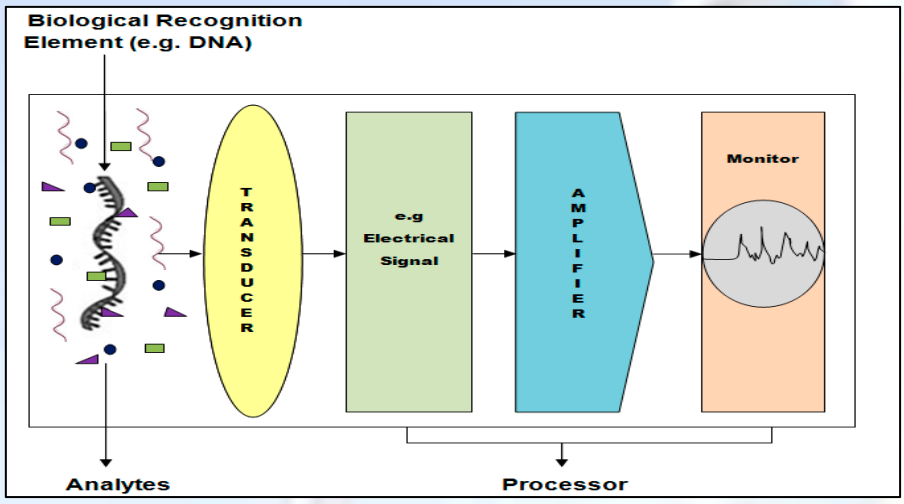

Fig 1. A schematic diagram showing basic biosensor assembly with a biological recognition element, transducer, and processor [1]

Working Principle of DNA Based Nanobiosensors

A biosensor is a device that detects, transmits and records the information on a biological analyte. Examples of analytes include nucleic acids (DNA, RNA), proteins such as enzymes, antibodies and antigens, or other biological component such as glucose. A basic biosensor assembly includes a biological recognition element, transducer, and processor[1].

- The DNA sample is collected from the patient.
- The biological recognition element, such as nucleic acids, antibodies, enzymes, proteins or whole cells can be integrated with a transducer via immobilisation, by covalent interaction, cross-linking or adsorption.
- The transducer converts the molecular biological signal into a digital or electric signal which is proportional to the concentration of the analyte.

- The detector element traps the signals from the transducer. These signals can be optical, electrochemical or magnetic signals [2].
- These signals are then passed on to the microprocessor where they are amplified and analysed.
- The data is then transferred to user friendly output and displayed or stored on the monitor.

Applications of DNA Based Nanobiosensors

1. Diagnosis of Genetic Diseases
2. Detecting Immunodeficiency Related Diseases
3. Diagnosis of Neurological Diseases
4. Detection of Infectious Diseases
5. Detection of Cancer

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Aindrila Indra
4th Year

Application of biosorption for removal of heavy metal from water

INTRODUCTION

With the growth of the industrial world, environmental challenges have also increased. A common type of pollution the world is currently struggling with is water pollution.

Heavy metals are removed from industrial wastewater by conventional methods such as reverse osmosis, electrodialysis, ultrafiltration, industrial ion exchange process and chemical precipitation. These common industrial methods of heavy metal removal have several disadvantages such as being expensive, requiring high amounts of energy, not appropriate for

removal of heavy metals at low concentrations. Biosorption methods are considered sustainable and more efficient in removal of heavy metals from aqueous media.

BIOSOPRTION

Biosorption is a biological physico-chemical process in which a biological material, such as plant biomass or microorganisms, is used to absorb or adsorb a target species, such as metal ions or dyes. In a biosorption process, two phases are present, a solid phase which it is referred as the biosorbent (e.g., plants, bacteria and fungi) and a liquid phase which is usually aqueous and contains the metal ions which are known as the sorbate. Algae, bacteria, fungi and plants are the most common biosorbents used for the removal of heavy metals from aqueous media. The main biosorption site of the biological sorbents is their cell wall. The cell walls of different biosorbents contain a range of different functional groups that contribute in biosorption process, the possible functional groups which are capable of biosorbing heavy metals are hydroxyl (found in alcohols and carbohydrates), carboxyl (found in fatty acids, proteins and organic acids), amino (found in proteins and nucleic acids), ester (found in lipids), sulfhydryl (found in cysteine (amino acid) and proteins), carbonyl (can be terminal such as in aldehydes and polysaccharides, or internal such as in ketones and polysaccharides too) and phosphate groups (found in DNA, RNA and tissue plasminogen activator). The functional groups of a biosorbent contributing in the removal of a specific metal can be studied and analysed using several analytical methods such as titration, infrared spectroscopy.

The potential of biosorption of a metal ion by a biosorbent is evaluated by the biosorption capacity value and equilibrium time for the biosorption process. Biosorption capacity is calculated according to the following formula:

$$q_e=(C_0-C_e)V/W$$

where q_e is the biosorption capacity (in mg of metal/g of biosorbent), C_0 and C_e are the initial and equilibrium concentration of metal ion solution (in mg/L) respectively, V is the volume of metal ion solution (in L), and W is the amount of biosorbent material dose used (in g). The higher the biosorption capacity, the higher the amount of heavy metal ion(s) a biosorbent can biosorb. Under optimum pH of media and temperature, the maximum biosorption capacity can be achieved.

MECHANISMS OF BIOSORPTION

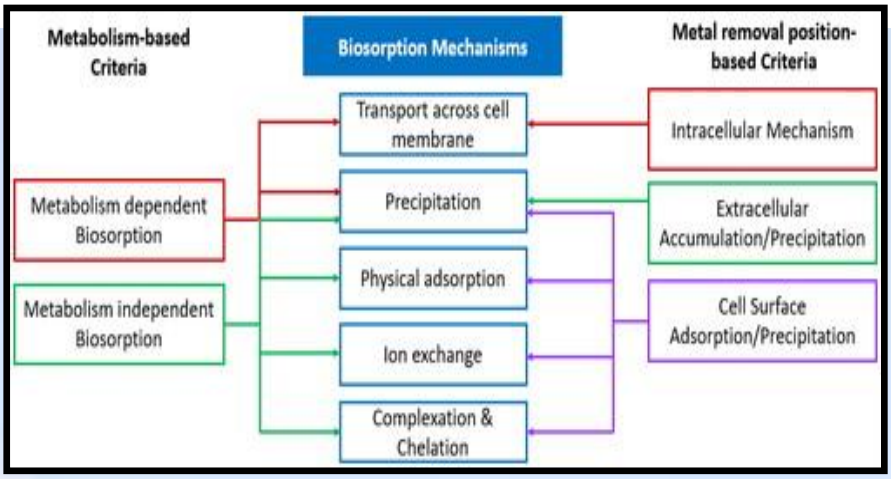

Figure 1. Classification of Biosorption Mechanisms

CONCLUSIONS

Biosorption methods can be an alternative to the common industrial methods of removal of heavy metals due to being environmentally friendly and sustainable for use. Several types of biosorbent materials can be used such as algae, bacteria, fungi and plants. Biosorption process can take place by several mechanisms including physical adsorption, ion exchange, complexation, precipitation and transport across the cells. The biosorption capacity of biosorbents can be affected by the pH of the environment, temperature, contact time, biomass dosage, initial metal concentration and other factors. A major limitation of the researches conducted in this area, studying the biosorption capacity of different biomass, is that they did not encounter for the complexity of real-life contaminated water.

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biosorption from Cu(II)-Co(II) single and binary mixtures on brown algae C. indica. *Journal of Environmental Chemical Engineering*.

Arka Das Karmaka
B. Tech 4th year

A review on the use of Zeolite Imidazole Framework-67 (ZIF-67) as a heterogeneous catalyst to activate peroxymonosulphate for degradation of organic dye like Rhodamine B (RB) in water

Synthetic dyes are widely used for coloring in clothes, leather accessories and furniture. Wastewaters from textile, dyeing and finishing industries are known to contain large amount of dyes, suspended solid particles and organics. Dyes present in this wastewater are a main source of water pollutant as they are resistant to biological degradation and are carcinogenic in nature. In this regard, there is a need of their removal in order to reduce pollution in the environment. Several processes such as adsorption, reverse osmosis, membrane separation, coagulation-flocculation, ion-exchange [resin], advanced oxidation processes has been used for treatment of wastewater. However, these processes posses some difficulties in process and operational conditions and thus, have limited capability for removal of dyes.

Photocatalysis, another widely accepted method for wastewater treatment, posses significant potential to degrade industrial dyes. Photocatalysis is the irradiation of light on a semiconductor that results in jump of electron from valance bond to conduction bond. The electron-hole pair formed reacts with oxygen and water to form superoxide anions and hydroxyl radical that has significant oxidizing ability for degradation of industrial dyes.

Sulphate radical (SO_4^-), generated from peroxymonosulphate (PMS) under UV irradiation have high oxidizing performance and reacts with other organic compounds to degrade wide variety of water pollutants. Sulphate radicals are preferred more over hydroxyl radicals due to its higher standard reduction potential (2.6-3.1 V). Sulphate radical suppresses the recombination of electron and holes and thus, enhances the degradation of industrial dyes.

Metal organic frameworks (MOFs) are compounds consisting of central metal ions coordinated to organic ligands to form three dimensional structures and are prepared by combining different metal ions and ligands. They are highly porous in nature and proven to be promising materials in hydrogen storage, CO_2 cature, catalysis, separation etc. Non-noble

metals such as cobalt, iron, copper, zinc, are used preparation of MOFs. A lot of these MOFs are used for degrading organic pollutants for wastewater treatment. MOFs, having transitional metal species, used as photocatalyst activates oxidising agent(PMS) by generation free radicals under UV irridiation. Earlier studies shows that transitional metals such as Fe $^{2+}$and Co^{2+} had been used for activation of PMS for degrading organic pollutants. But the use of metal ions in homogenous phase leads to loss of metal and thus there is a need of using heterogenous transition metal based catalyst for activation of PMS. Considering that cobalt is proven as the most common and effective catalyst for PMS, a cobalt-based MOF, Zeolitic Imidazole Framework (ZIF)-67, is used to degrade a cationic dye, Rhodamine B (RB) in water. ZIF-67 is prepared by reacting cobalt ion and 2-methylimidazole (2-MIM).

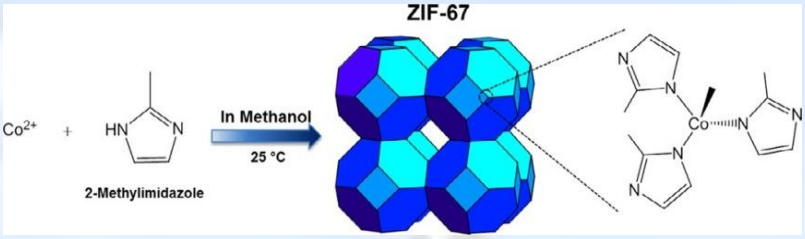

Fig. 1. Synthesis of Zeolitic Imidazole Framework (ZIF)-67 [4]

The presence of ZIF-67 facilitates the activation of PMS to generate sulfate radicals which helps in degradation of RB. The cobalt ion in ZIF-67 can exchange state between Co^{2+} and Co^{3+} after adsorption and desorption of external molecules (*e.g.*, oxygen) in water. Cobalt ions reacts with PMS to generate sulfate radicals as follows (Eqs 1 and 2):

$$Co^{2+}@ZIF{-}67 + HSO_5^- \rightarrow Co^{3+}@ZIF{-}67 + SO_4^{\bullet -} + OH^- \quad (1)$$

$$Co^{3+}@ZIF{-}67 + HSO_5^- \rightarrow Co^{2+}@ZIF{-}67 + SO_5^{\bullet -} + H^+ \quad (2)$$

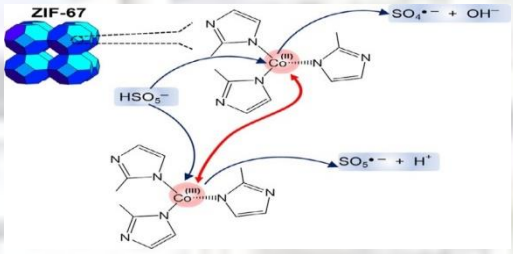

Fig. 2. Mechanism using ZIF-67 to activate peroxymonosulfate(PMS) [4]

While ZIF-67 shows its promising potential as a heterogeneous catalyst for the PMS activation, it also reveals that ZIF-67 can be used continuously for multiple cycles with stable and effective catalytic activity as shown in Fig.3.

Increasing ZIF-67 loading enhances the degradation kinetics and extent significantly. The higher temperature also led to the faster degradation kinetics and extent. The RB degradation using PMS activated by ZIF-67 can also be enhanced by the UV irradiation and ultrasonication. These features make ZIF-67 an interesting and promising heterogeneous catalyst to activate PMS for the degradation of organic pollutants in water.

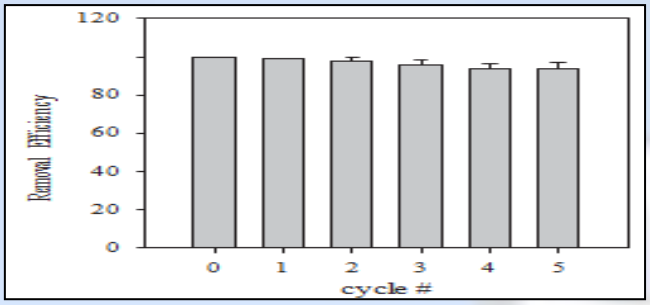

Fig. 3. Recyclability of ZIF-67 [4]

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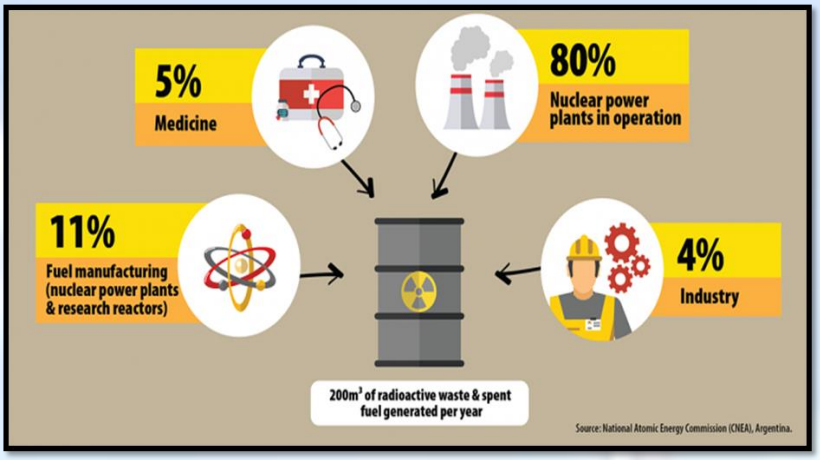
Niladri Poddar

4th Year

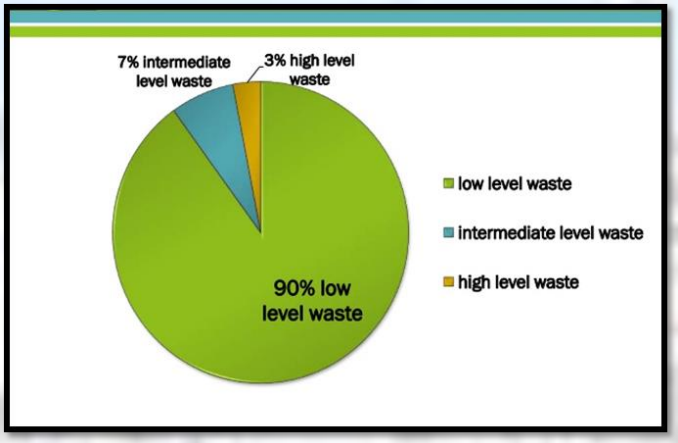
RADIOACTIVE WASTE MANAGEMENT

INTRODUCTION-Waste materials containing radioactive material emitting alpha, beta and gamma rays by the impact of neutrons are called radioactive wastes. Rate of decay of these wastes are calculated by half-life, ^{238}U having the largest half-life of 4.5 billion years. These are the byproducts of nuclear power generation which are hazardous to humans and environment, so must be properly disposed.



Radioactive wastes can be generated form nuclear fuel cycle operations, industry, nuclear weapon reprocessing, defense and medicine and naturally occurring radioactive material.

TYPES OF RADIOACTIVE WASTES- There are 3 types of radioactive waste based on hazardousness- 1. *Low level waste*, 2. *Intermediate level waste*, 3. *High level waste*.



Low level wastes are found in medical wastes, rags from fuel cycle buried at 30m depth below ground. Intermediate wastes are found in reactor's metal cladding and need more isolation. High level wastes are formed by burning uranium fuels and are deadly for humans. [1]

MANAGEMENT PROCESSES- **1. Spent Nuclear Fuel Pool** contains cooling water kept over heated nuclear spent fuel which are HLW. These are 7-12 meters deep made of concrete. After fuel is cooled they are stored underground as deep geological repository described next.

2. Deep geological repository is a common method having series of barriers naturally existing or technically built so that the radioactive waste storage is not affected by human activity. This is done at least 200m below earth's surface.

TREATMENT PROCESSES OF WASTES-

1. **Radioactive waste transmutation** is where radioactive isotopes are converted into non-radioactive isotopes by fission reaction, destroying original harmful actinide isotope in a critical reactor by a photon beam from accelerator. [2]

2. **Vitrification** is a process where HLW is treated with sugar and then calcined at 1000˚C to remove all moisture. Liquid wastes are transformed to solid matrix by incorporating into

molten glass. This solid can be then stored in geological deposit in steel cylinders. The figure below shows a part of vitrification plant in Trombay, India. [3]

CONCLUSION-Following the rules and regulations of radioactive waste management, public and the environment will be safeguarded. Recent explosions in Lebanon has shown what happens if wastes are not properly managed. India has achieved self-reliance in the management of many types of radioactive waste. In line with global scenarios, technologies are constantly upgraded.

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TANMAY PAUL (CHE, 4th YEAR)

Mathematical Modeling of Lactic Acid Production and Preservation of Milk

INTRODUCTION: Liquid milk and dairy products have been an important nutrient source for a thousand years for building healthy bones and for maintaining a healthy weight. This study is carried out to analyse methods of milk processing and preservation. During storage and distribution, milk is exposed to a wide range of environmental conditions and can be affected by microorganisms, which may lead to milk quality deterioration. This study also explains the kinetic analysis and mathematical modeling of growth and lactic acid production of *Lactobacillus casei* in deproteinized and nonsupplemented milk.

MATHEMATICAL MODEL: Analysis of biomass, substrate and product time profiles:

$$r_X = d[X]/dt = \mu [X] \quad \ldots\ldots\ldots (1)$$

$$r_P = d[P]/dt = \alpha r_X + \beta [X] \quad \ldots\ldots\ldots (2)$$

$$r_S = -d[S]/dt = \left(1/Y_{X/S}\right) r_X + \left(1/Y_{P/S}\right) r_P \quad \ldots\ldots\ldots (3)$$

Where, r_X = biomass production rate

[X] = biomass concentration (○)

r_P = lactic acid production rate

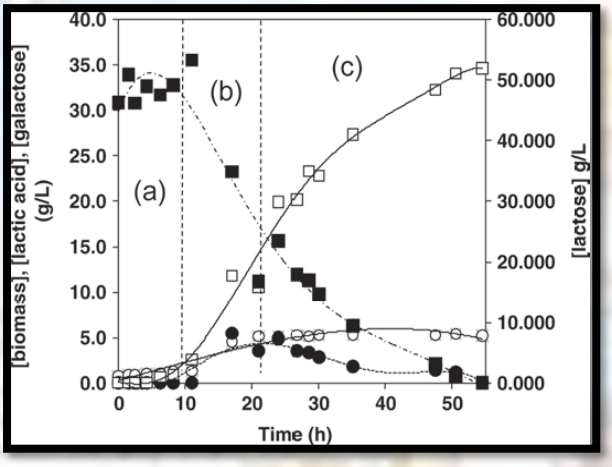
[P] = lactic acid concentration (□)

r_S = lactose concentration rate

[S] = lactose concentration (■)

$(Y_{X/S})$ = biomass/substrate yield coefficient

$(Y_{P/S})$ = product/substrate yield coefficient

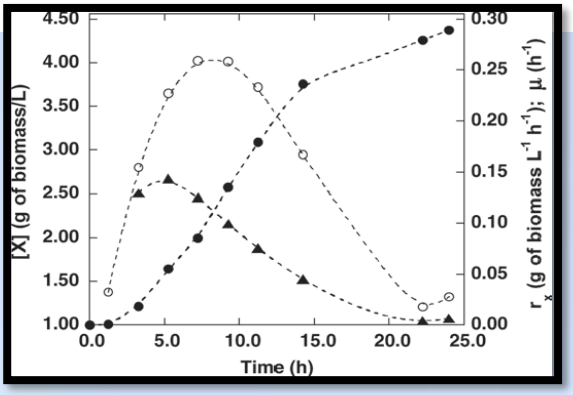


Rates are analysed to infer relationship between substrate, product and biomass concentration. The plot is segmented in three fermentation stages: a) An extended lag phase, b) A phase of exponential biomass growth and lactic acid production, c) A stage, where lactic acid continues to be produced but no further biomass growth is observed. To kinetically analyse the processes of *Lactobacillus casei* growth, the experimental biomass concentration profile to a fourth-order polynomial trend was fitted where a, b, c, and d are polynomial coefficients:

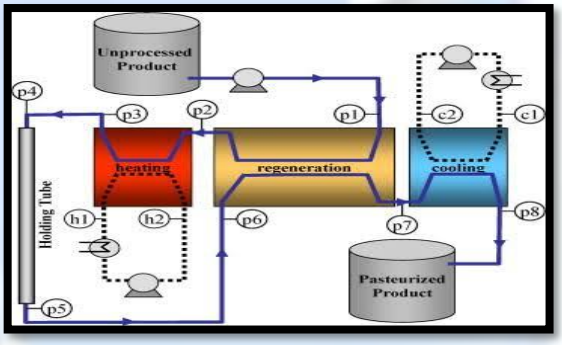
$$[X] = a + bt + ct^2 + dt^3 \quad \ldots\ldots\ldots (4)$$

$$r_X = d[X]/dt = b + 2ct + 3dt^2 \ldots\ldots\ldots (5)$$

$$r_X = \mu [X] \text{ then } \mu = (b + 2ct + 3dt^2)/[X] \ldots\ldots\ldots (6)$$



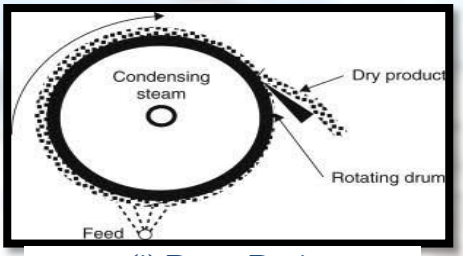
During the early stage of exponential growth, specific growth rate, (μ, ▲) reached its highest value. However, after 5 hours it started decreasing substantially because the biomass concentration ([X], ●) increased with time. Biomass production (r_X, ◌) was also at its peak. [1]



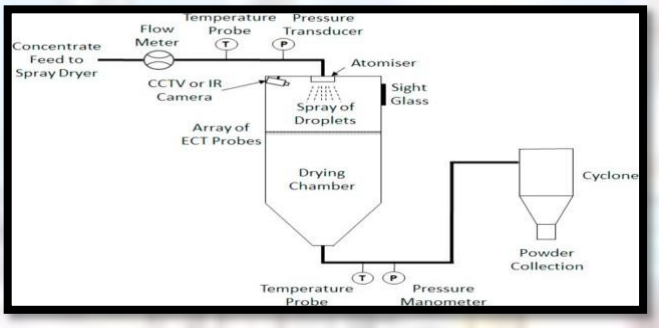
PRESERVATION:

Pasteurization: Milk is heated to a specific temperature, then followed by cooling which destroys only vegetative form of bacteria and the spores survive. Types: (i) HTST Pasteurization (Temperature is maintained at around 70˚C for about 15-30 secs.), (ii) LTLT Pasteurization (at 65˚C for 30 mins.), (iii) UHT Pasteurization (at 138˚C for min. of 2 secs.).

Sterilization: This process kills all forms of microbial lives including fungi, bacteria, viruses, spores etc. Types: (i) Physical, (ii) Chemical (iii) Irradiation and (iv) Filtration. **Dehydration:** This process generally forms milk



(i) Drum Drying



(ii) Spray Drying

powder because it has far longer shelf life than liquid milk. [2]

CONCLUSION: In summary, temperature of milk has a significant effect on the rate of bacteria development and consequently spoilage of milk. Besides, from the kinetic analysis, we have seen the strong inhibitory effect of lactic acid on biomass growth rate as well as the exponential decay of specific growth rate due to lactic acid accumulation.

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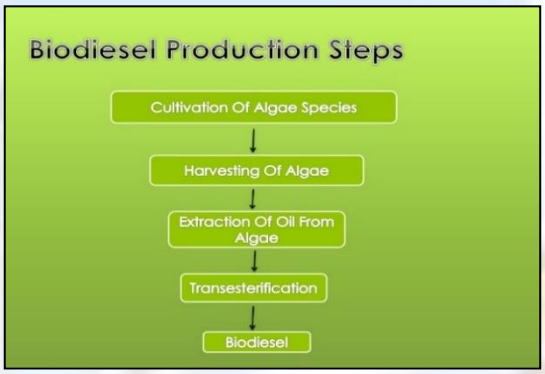
SRIJITA DE,
ChE, 4th YEAR

PRODUCTION OF BIODIESEL FROM ALGAE

BIODIESEL: Biodiesel is the monoalkyl esters of long-chain fatty acids which is derived from transesterification of biological matter. It is an excellent renewable and safe alternative fuel with environment friendly nature.

MECHANISMS OF OIL PRODUCTION:



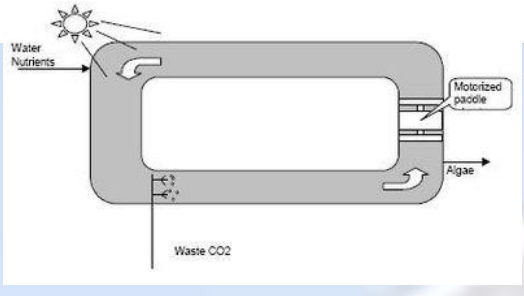
- Selecting the best algae
- Large scale production
- Cell disruption
- Solvent extraction
- Trans-esterification for biodiesel production
- Production of green-diesel by de-carboxylation or hrdrogenation

SELECTING THE BEST ALGAE: Spirogyra is the most common green algae, available abundantly in springs, ponds and brackish water. It produces lipids, carbohydrates and proteins that can be utilised for the production of biodiesel.

LARGE SCALE PRODUCTION OF ALGAE: Algae can be cultivated in two ways—in an open pond system (natural or engineered) or closed system.

- **Open pond systems:** Open ponds have a variety of shapes and sizes but the most commonly used design is the raceway pond. Open ponds are easy to maintain since they have large open access to clean off the biofilm that builds up on surfaces. The disadvantage of open systems is that by being open to the atmosphere, they lose water by evaporation at a rate similar to land crops and are also susceptible to contamination by unwanted species.

- **Photobioreactors:** Closed photobioreactors provide sterility and allow for much greater control over culture parameters such as light intensity, carbon dioxide, nutrient levels, and temperature. Under optimal conditions, microalgal populations are capable of doubling within hours and achieving high cell densities

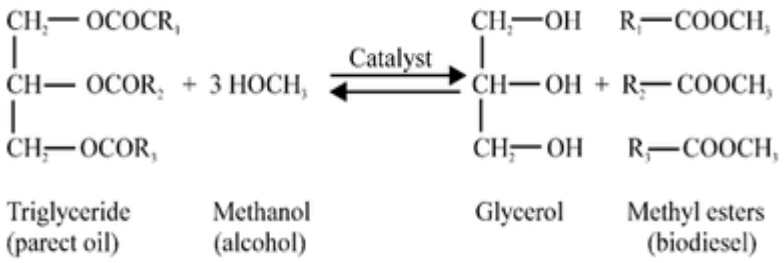


ISOLATION OF OIL:

- **CELL DISRUPTION:** Mechanical disruption of algal cells aims to damage cell walls to provide access to the intracellular content . Disruption methods avoid use of chemicals and contamination of the left over biomass, leaving the extracted biomass for further product development (e.g., high protein animal feed etc.). Common methods include bead milling, homogenization, and mechanical pressing .
- **SOLVENT EXTRACTION:** Solvent extraction makes use of specific chemicals to extract the lipids and separate them from the crude biomass. Possible solvents for extraction include benzene, isopropanol, ethanol, and hexane or ethanol-hexane mixtures.

TRANS-ESTERIFICATION FOR BIODIESEL PRODUCTION:

Biodiesel production from microalgae can be done using several well-known industrial processes, the most common of which is base catalyzed transesterification with alcohol. The transesterification is the reversible reaction of fat or oil (which is composed of triglyceride) with an alcohol to form fatty acid alkyl ester and glycerol. Stoichio-metrically, the reaction requires a 3:1 molar alcohol to oil ratio, but excess alcohol is (usually methyl alcohol is used) added to drive the equilibrium toward the product side . This large excess of methyl alcohol ensures that the reaction is driven in the direction of methyl esters, i.e. towards biodiesel. Yield of methyl esters exceeds 98% on a weight basis. The reaction occurs stepwise: triglycerides are first converted to diglycerides, then to monoglycerides and finally to glycerol. Consequently, alkalis such as sodium and potassium hydroxide are commonly used as commercial catalysts at a concentration of about 1% by weight of oil. Alkoxides such as sodium methoxide are even better catalysts than sodium hydroxide and are being increasingly used.



DE-OXYGENERATING FATTY ACID FOR GREEN DIESEL

Trans-esterification leads to presence of oxygen hence biodiesel is not a direct substitute of diesel which are actually medium to long chain unbranched alkanes.

Pyrolytic cracking or hydrogenation could address to the problem but it might produce fuels with low energy content.

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SRIJIKA BANERJEE

4th year

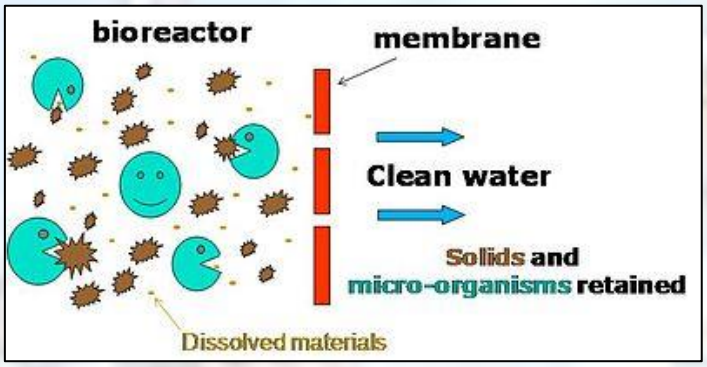
MEMBRANE BIOREACTOR FOR WASTE WATER TREATMENT

INTRODUCTION: Wastewater treatment is the process of converting wastewater – water that is no longer needed or is no longer suitable for use – into bilge water that can be discharged back into the environment. Wastewater is full of contaminants including bacteria, chemicals, and other toxins. Its treatment aims at reducing the contaminants to acceptable levels to make the water safe for discharge back into the environment. There are two wastewater treatment methods namely chemical or physical treatment methods, and biological wastewater treatment methods. Biological waste treatment process (Activated sludge process) use biological matter and bacteria to break down waste matter. Alternatively, physical waste treatment methods use chemical reactions as well as physical processes to treat wastewater. Membrane bioreactor (MBR) technology, which combines biological-activated sludge process and membrane

filtration has become popular, abundant and accepted in recent years for the treatment of many types of waste waters, whereas the conventional activated sludge process (CAS) process cannot cope with either composition of wastewater or fluctuations in wastewater flow rate. MBR technology is also used in cases where demand on the quality of effluent exceeds the capability of CAS. MBRs have been used for both municipal and industrial wastewater treatment and reclamation.

MEMBARNE BIOREACTORS: An **MBR** is a hybrid of a conventional biological treatment system and physical liquid–solid separation using membrane filtration in one system. Membrane bioreactors for wastewater treatment are a combination of a suspended growth biological treatment method, usually activated sludge, with membrane filtration equipment, typically low-pressure microfiltration (MF) or ultra filtration (UF) membranes. The membranes are used to perform the critical solid-liquid separation function. In activated sludge facilities, this is traditionally accomplished using secondary and tertiary clarifiers along with tertiary filtration.

An MBR, or Membrane Zone, can best be described as the initial step in a biological process where microbes are used to degrade pollutants that are then filtered by a series of submerged membranes (or membrane elements). The individual membranes are housed in units known as modules, cassettes, or racks and a combined series of these modules are referred to as a working membrane unit. Due to the fact that the membrane pore size may be below 0.1μm, MBR can effectively produce a high-quality clarified effluent. Membrane filtration ensures that microorganisms are completely trapped into the bioreactor and this gives better control over the biological reactions and modifying the conditions of the microorganisms in the aerated tank.

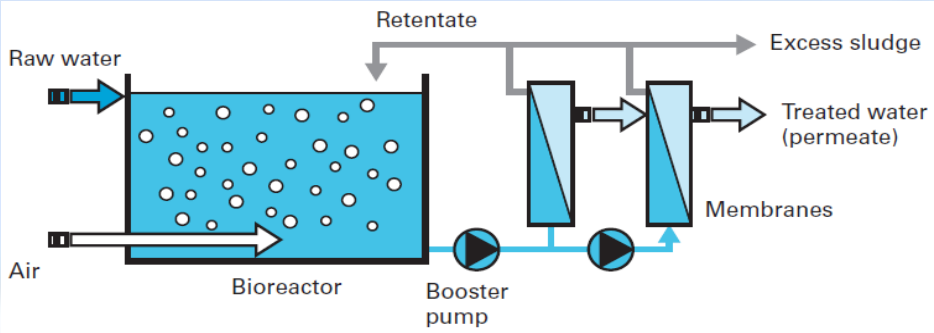


A membarane bioreactor

WORKING THEORY: It occurs in the following steps:

- **Screening stage**, where the heavy solids and larger molecules (scrum and grit) are separated, so that these do not trap the surface of the membrane and no fouling occurs.

- **Biological process** involving vigorous agitation due to air bubbles generated from blower system. This acts to scour and clean the surface of membrane to prevent build-up of material and also to provide sufficient oxygen concentration for biological action.
- After this, the wastewater is passed through membrane whereby the **permeate** (treated water) is obtained and the **retentate** (including solids) are returned back to the system.



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SOUBARNO SEN
4th Year

APPLICATION OF METAL-ORGANIC FRAMEWORKS (MOFs) IN CARBON DIOXIDE CAPTURE

The climate change observed in the recent years, caused mostly by global warming, is the subject of a widespread global concern. The CO_2 emission associated with anthropogenic activities plays a big role in the global warming and climate change. The main contributors to the observed CO_2 emissions are – vehicular emissions, fossil fuel-fired power plants, deforestation and chemical processes. Figure (a) represents how the atmospheric CO_2 concentration increases with increase in human emissions. About a 50% increase in the CO_2 emission is expected by fossil fuel-fired power plants alone by 2030.

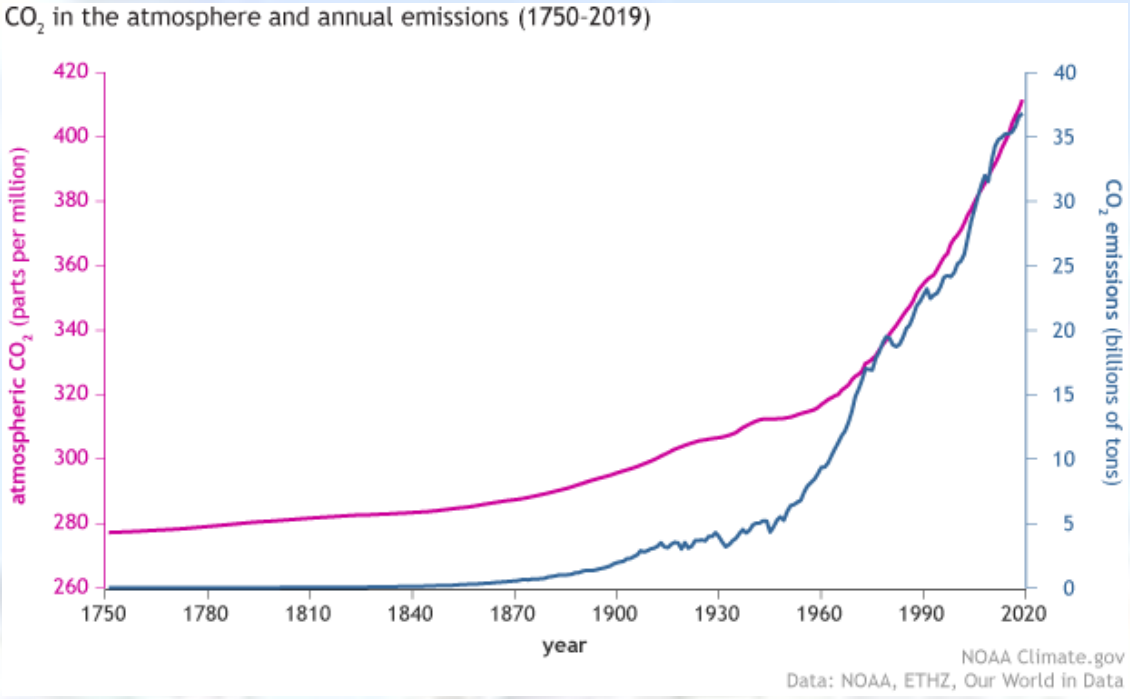

Fig. (a) Increase in atmospheric CO_2 with increase in human emissions [1]

Therefore extensive research efforts have been taken worldwide to develop feasible materials for CO_2 capture. Various capture routes has been developed, with post-combustion capture being recognised as the most mature and flexible one. Due to various process challenges, adsorption by solid materials is being considered as it has benefits of low energy requirements, low capital and operating costs and reduced secondary waste generation. Metal-organic frameworks (MOFs) have come across as promising candidates for CO_2 capture and storage on account of its large surface area, high porosity and structures that can be tuned as per requirement. MOFs are a novel class of crystalline porous materials having one-, two- or three dimensional structures consisting of metal ions at the nodes and organic groups linking the

metal nodes. Researchers have synthesized MOFs that feature a surface area of more than 7000 square metres per gram [4]. By making the MOF from different metal atoms and organic linkers we can create materials that can be used to adsorb specific gases or in other applications which include gas purification, in catalysis and also in controlled drug delivery systems. Due to its vast applications MOFs have become the fastest growing class of materials today. More than 20,000 MOFs have been fabricated and synthesized in the last decade. MOF-5 [$Zn_4O(BDC)_3$] is one of the initial metal-organic framework that had been reported in the year 2000 by Dr. Omar M. Yaghi and his team. Fig. (b) Shows an unit cell structure of MOF-5 in which the yellow sphere represents the volume of the pore. Oxygen in red, carbon in black, hydrogen in white and the tetrahedrons represent the coordination of BDC (1,4-benzodicarboxylate) to the zinc centre.

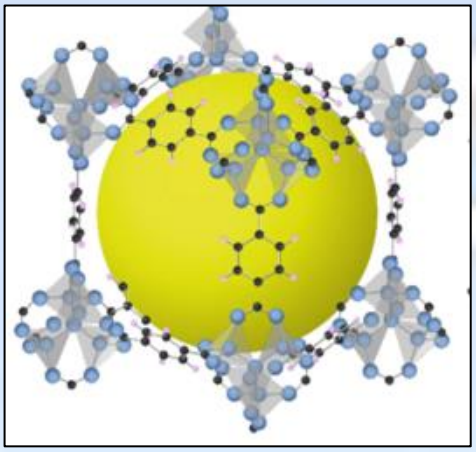

Fig. (b) Unit cell structure of MOF-5

Researches in MOFs are still in its early stages so, experiments are laboratory scale and are employed in the form of packed bed adsorption where, the MOF adsorbents are packed in the form of pellets. After the packed bed is saturated with CO_2, the CO_2 can be released in a pure stream either by increasing temperature in a temperature swing adsorption (TSA) or by decreasing pressure in a pressure swing adsorption (PSA) [5]. For post-combustion capture TSA might represent a more feasible process since the flue gas is released at ambient pressure. Due to the freedom that MOFs offer with respect to optimization as per requirement they are worthy candidates in environmental applications and they might help us in solving this crisis that the world is currently facing and can turn out to be a boon for mankind.

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Somantika Pradhan

4th year

Drug formulation - Discovering drugs for the future

The use of drugs for improving life expectancy and curing diseases has been known since ages however little was known about the backend process of drug formulation. This pandemic made me curious about drugs, so I explored various stages and processes of drug formulation.

The pharma and biotech industry

The pharmaceutical and biotechnology industry produces drugs and other products that help people and animals live healthier lives, recover from injuries, and fight illnesses. It is home to cutting-edge biological and chemical research and offers opportunities for people across a wide spectrum of careers from scientists, physicians, and engineers to marketing and sales workers and human resources professionals. The advancement of a new medicine starts when scientists study a biological target (e.g., areceptor, enzyme, protein, gene, etc.) that is involved in a biological process thought to be dysfunctional in patients with a disease. Here, we are considering the discovery and development of entirely new medicines, those with a mode of action different from already approved medicines, and intended for a clinical indication that is not addressed by approved medicines. Better medicines that are an iterative enhancement on current medications are advantageous as they may offer benefits over existing medications in terms of potency, safety, tolerability or convenience, but they usually do not involve the manipulation of biological targets different from those directly affected by existing medications. Analysis across all therapeutic areas indicate that the development of new medicine, from target identification through marketing approval, takes over 12 years and often much longer. The cost to develop a new molecular entity is undoubtedly over $1 billion and on average, has been estimated to be about $2.6 billion. This is based on investigation across several therapeutic areas and includes data from development programs that are new iterations

of existing medicines as well as those medicines based on entirely new targets or that aim for completely unprecedented therapeutic indications. Data from public health laboratories and public health policies are also used to formulate drugs. The probability of advancing a drug candidate is very low. For an instance, scientists start with around 100 molecules which have the potential to have a biological impact on the target site. Out of them, only a few get approved and only a fraction of the approved make their way to the drug. Therefore, a very large number of biological targets are discovered and interrogated pharmacologically and genetically to achieve a single new disease-modifying medicine.

Key issues for pharma

To develop a drug, the company order their scientists to carry out research and development projects. While developing drugs scientists keep in mind that drugs which are expensive and marginally better than existing drugs are less likely to attract customers because people pay premium only if the drug is first in class or the best in class. For this, the company needs to be fast enough to launch a drug in the market and acquire its patent or improve the existing drug significantly. The R&D process takes about 10- 12 years and time is very important in the pharma industry as patents are valid for 20 years. Thus, a company has hardly 7 -8 years to generate profits from the drug because after that it becomes a generic drug. Also, the research and development part require huge capital investments and time. The odds of a drug making it to the market can be as low as 6% with more than $100 billion being spent on R&D and comparing this amount to the success rate we can see that only $10 billion is producing fruitful results rest all goes into vain.

Other challenges include lack of proper skilled employees in the desired number, drug regulations changing all over the world, the time required for drug approval (min. 2.5 to 3 years), changing healthcare system from product-centric to patient and payer centric. The funding allocated to different projects in research and development is based on some predictions and criteria. The drugs for the younger generation are given more importance compared to the drugs for the older generation as youngsters are expected to live longer. Moreover, the future diseases are predicted and drug formulation is progressed based on current abnormalities and variations. As mentioned earlier, general health surveys on people of various age groups is detrimental in designing drugs for the future. A survey of people aged from 30 – 40 years over 5 years showed an increased tendency of higher cholesterol levels and at the same time, people of this age group were seen to have comparatively increased heart problems. Research showed that cholesterol has tremendous effect on heart health, so the pharma predicted in the upcoming years, people have an increased risk of higher cholesterol levels, so

they started inventing drugs to lower the cholesterol levels. Some pharma companies use this survey unconventionally. One such example is of CIPLA pharmaceuticals. Many future diseases were predicted from almost every part of the body but CIPLA chose to specialize on manufacturing drugs for respiratory illnesses instead of formulating drugs for multiple diseases. This helped CIPLA to capture the majority of the respiratory drug market in India.

These surveys and researches are helpful yet in another way. It helps in combating unforeseen outbreaks and pandemics. In case of a sudden outbreak, it is not possible to develop a drug specific to the disease. The scientists try to find out the cause of the disease and the family of microorganisms to which it belongs so that patients can be treated with the existing drugs in the market. To simplify this, let's take the example of COVID – 19. This coronavirus is not a new virus, it belongs to the category of SARS viruses known to cause the acute respiratory syndrome. There have been outbreaks of this class of virus earlier however they did not turn into a pandemic. The crown-like structure on coronavirus is what makes it lethal as it uses this crown to stick to surfaces for a longer period. So, we see here that coronavirus is a mutation of the already known virus, therefore similar doses of medicines are used in combating this class of virus and body's response is monitored. When the patients are seen responding to the existing drugs, it buys some time and gives idea to the pharma companies to develop drugs specific to the disease. For manufacturing drugs, the disease is chosen for which the drug has to be made followed by critical examination of the target molecules on which the drug molecules will produce their effect. The key of drug formulation is to integrate the biology standpoint with the chemical synthesis standpoint. Not all drugs are a new invention, sometimes they are made to replace the drugs present in the market. This is a cheaper option compared to its alternative. Drugs that replace existing drugs in the market are developed with the idea that they will have higher efficacy compared to the existing drugs or cheaper than its counterparts or both. Another point here is that they have to ensure that they are building a robust drug molecule which complies with the latest standards of safety and produces the desired benefits. This is followed by testing the drug and measuring the highest dose which the body can tolerate. We track the response and side effects of the drug by starting with a single dose and then extend the observation time to the estimated time of recovery of the disease by testing it on animals. For example, if the new medicine is given to a rat, we give it a single dose, wait for a response and if it's the desired response, we continue the dose given to these animals periodically until it shows a reproducible effect in a dose-responsive manner in this efficacy model. Safety nowadays comes above just about everything else here. All the results

and trials are closely documented to prove the overall safety of a drug. After a drug clears all the clinical trials both in humans and in animals, the drug is commercialized.

Commercialization of drugs

We need to understand the basic business models in the industry to commercialize drugs. The pharma industry has 3 major business models: innovator, generic, and over-the-counter drugs. The innovator model is all about new chemical and biological entities, which includes high R&D investments. The revenue in this model is only generated during its patent life after which the generic companies capture the market. Generic makes copies of the drugs after the patents expire. These are cheaper than the innovator's version as they come with a discount range of 10% to 95%. Third, we have the OTC or over the counter drugs. They also produce generic drugs but with a very safe product profile and the patient can obtain the drug without a prescription. To understand this, let's take the example of LAMISIL, a drug used to cure athlete's foot-launched by Novartis. It was a great prescription drug that ruled the market during its patent life. After its patent got over then the drug was launched in OTC form in various forms like topical creams and lotions. Over the counter drugs involve direct consumer marketing. Therefore, the labels and physical appearance of the packaging matters in determining its overall sales. Since every business model has certain limitations fueling the pipeline is very important to keep the business running. For the innovator model, continuous research and development are necessary for fueling the pipeline without which the company would be unable to survive in the market. For generic, it is the production of drugs at reasonable costs and for OTC it is direct consumer marketing. Another aspect of drug commercialization is selling the drugs in the market which the companies have produced. It is a common trend that the majority of the drugs invented are launched in the USA first. This is because the FDA has no legal authority to regulate drug pricing. So, the companies can charge the highest amount the customers are willing to pay for plus an additional 10% of the price. This is one of the reasons why healthcare is expensive in the USA. The European Union has certain regulations for drug pricing to prevent exorbitant pricing of drugs. So, if a drug in the US market is launched at a higher price, the same drug will be launched at a reduced price in Europe. So, they can still earn a decent margin but it will not be the case if it is launched in Europe first because if the ceiling price is already low then it isn't possible to be priced higher than that. In this way, drugs finally reach us after its formulated and tested.

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Sushmit Ghosh
2nd year CHE

Making thermoset plastic recyclable

The NCERT definition of thermoset plastic say that these are polymeric material that cannot be recycled once moulded to a particular shape however this definition is about to change as scientist have now developed a way to modify thermoset plastics using the industrial thermoset **poly-dicyclopentadiene** as a model system.

Thermoset plastics contain polymers that cross-link together during the curing process to form an irreversible chemical bond. They play a key role in the modern plastics and rubber industries, comprising about 20 per cent of polymeric materials manufactured today, with a worldwide annual production of about **65 million tons**

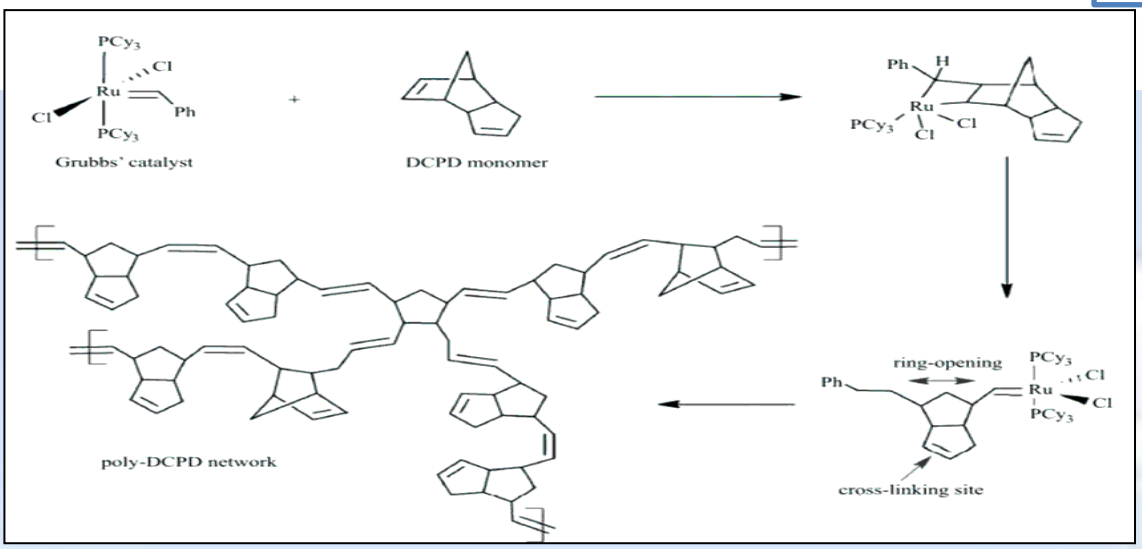
The high density of crosslinks that gives thermosets their **useful properties** (for example, chemical and thermal resistance and tensile strength) making thermosets ideal for high-heat applications such as electronics and appliances.

However these very properties is the cause of one of its **major drawbacks** the strong covalent bonds do not allow the plastic to be easily recycled or broken down after use, because the chemical bonds holding them together are stronger than those found in other materials such as thermoplastics.

The Process to recycle:

Step-1:- Ring-opening metathesis polymerization (ROMP) a type of olefin metathesis chain-growth polymerization is used to add the 3rd generation **Grubbs catalyst** within the polymeric backbone of the structure.

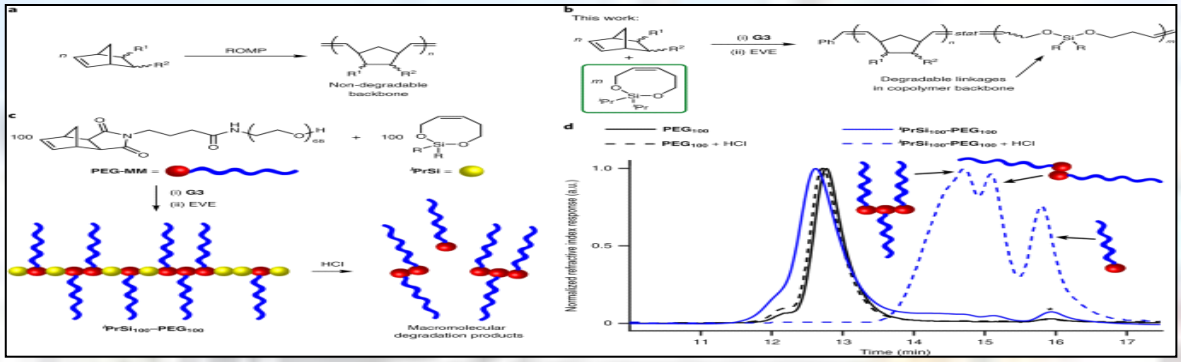
The mechanism for this reaction is similar to any olefin metathesis reaction where the redistribution of fragments of alkenes (olefins) takes place by the scission and regeneration of carbon-carbon double bonds.



Pictorial representation of the reaction

Step-2:- In this step, the **Silyl ether** (a monomer) is randomly distributed throughout the material forming 7.5 and 10 percentage of the overall material group as it replaces the Grubbs reagent in the **polymeric structure** of PDCP.

As a result, a small number of cleavable bonds are selectively installed within the strands of thermosets. Introduction of cleavable bonds within the strands of covalently cross-linked thermoset plastics can impart **degradability and potential recyclability** into the polymer



Addition of Silyl ether within the polymeric chain backbone

Step-3:- After adding cleavable bonds within the polymeric chain of the thermoset plastic. **Tetra butyl ammonium fluoride (TBAF),** a fluoride reagent that selectively cleaves Silyl ether (the monomer added) thus breaking the strong covalent bonds of the thermoset plastic.

The degradation products of iPrSi-doped pDCPD are hydroxylated polymers bearing cyclopentenadiene functionalities.

The greatest advantage of the technology:

After comparing the native material with the recycled one on various parameter like young's modulus , stress strain curve and impact resistance it was found out that the new material has nearly indistinguishable, and in some ways improved, mechanical properties compared to the original material.

Moreover, recycling of thermoset plastic saves the earth from millions of tonnes of plastic waste as well.

The recyclability of thermoset plastic in the next big innovation in the field of polymers this not only opens up new business avenues but helps to tackle the modern day problem of waste generation by plastics to some extent.

Industrial application

Since the research is still quite fresh the industrial impact that this technology can bring about is yet to be discovered however researchers are now hoping to form a company to license and commercialize the technology. SP insight, a USA based company has been performing some preliminary economic modelling and secondary market research. Leading industry players, say the technological advancement is good for stakeholders throughout the value chain. Parts fabricators get a stream of low-cost recycled materials. Equipment manufacturers, such as automotive companies, can meet their sustainability objectives; and recyclers get a new revenue stream from thermoset plastics.

Reference

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Vaibhav Arora
4th year