



Chemical Engineering Department-BIHE
Final Project for Bachelor's Degree

Two-Dimensional Nanomaterials in Water and Wastewater Treatment Processes

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Abstract

Activities such as household use, agriculture, and industrial processes are causing contamination of freshwater resources on Earth. This contamination poses risks to both aquatic bodies and human health, particularly from organic pollutants and heavy metals. Therefore, efficient treatment methods for industrial wastewater are crucial to address these serious threats. Following the primary and biological treatment steps, commonly used, cost-effective treatment methods include absorption, flocculation, and filtration to remove contaminants from wastewater. Recent advancements in 2D nanomaterials, such as graphene oxide, metal-organic frameworks, and molybdenum disulfide, offer unique structures and superior properties that can address major challenges in water treatment. These atomically thin materials have a large surface area and mechanical strength, making them suitable alternatives for existing desalination and water purification membrane materials. This research aims to explore the synthesis and application of various 2D nanomaterials in the final stage of wastewater treatment and their effectiveness in removing various contaminants from drinking water. The study also considers the commercial viability of 2D nanomaterials for these applications and the challenges that need to be addressed. Additionally, in this project, a water purification plant for the Persian Gulf region in the Salakh area has been designed, and an economic analysis of this type of material has been conducted.

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Chapter 1

Introduction

1.1 Introduction

Access to clean water is crucial for sustaining life on Earth. Research shows that only 28 percent of the global population have access to potable water, while 15 percent struggle with insufficient quantities to maintain a standard and healthy lifestyle. As a result, many people suffer from illnesses or even die due to the consumption of contaminated water. ⁽¹⁾

On the other hand, the continuous growth of the population, urban migration, urbanization, and the expansion of various industries contribute significantly to the generation of substantial volumes of wastewater, emerging as a significant environmental challenge. However, it's worth noting that this considerable amount of wastewater can serve as a valuable water source across different sectors. Therefore, treating contaminated water derived from diverse wastewater qualities becomes pivotal in ensuring a reliable industrial water supply. Water holds crucial importance in industrial processes, providing functions such as serving as raw materials, transportation, cleaning, and system cooling. It plays a key role in various industries, including chemical, metal, food and beverage, paper, and textile sectors. The emergence of industries and changing environmental conditions, such as climate change, have intensified the demand for daily water supply and investments in water treatment. Consequently, aside from conserving water resources, the efficient utilization of these resources and the adoption of

appropriate industrial water treatment systems can also contribute to reducing the overall costs within industrial systems. ⁽²⁾

Removing pollutants from the environment is challenging due to their persistent nature. Physicochemical and biological techniques are now used for this purpose. Physicochemical methods in wastewater treatment, including reverse osmosis, UV, ion exchange, and algal method, are common. However, these conventional approaches have their limitations. For instance, RO processes used to reclaim municipal wastewater face challenges related to handling the concentrated waste by-product (RO concentrate, which typically constitutes 10% to 50% of the original feed water), which can constitute a significant portion of the original feed water. Additionally, fouling of RO membranes remains a challenge. ⁽³⁾ Algae systems, while effective, require clear water to ensure optimal transparency for algae growth. ⁽⁴⁾ Additionally, UV disinfection, although useful, may lead to regrowth or photoreactivation of microorganisms after exposure to UV light. ⁽⁵⁾

As the industry seeks more sustainable and eco-friendly solutions, innovative technologies are being explored to tackle wastewater contamination. ⁽⁶⁾

In the 21st century, the field of water treatment has seen exciting advancements through nanoscience and nanotechnology. Different Nano systems, like zero-dimensional nanoparticles, one-dimensional nanowires/nanorods, two-dimensional nanoplates/nanosheets, three-dimensional nanostructures (Fig.1), and their functional composites, have captured attention in water treatment and monitoring. Among these, 2D nanomaterials (2DM) are considered the thinnest with potentially the largest surface-to-volume ratio. This suggests minimal material usage, quick processing, and highly efficient treatment. The unique shape of 2D nanomaterials also gives them distinctive physical and chemical properties ⁽⁷⁾ like high anisotropy, effective surface area, mechanical strength, plasmonic, electron confinement, and optical properties (Fig.2). ⁽⁸⁾ compared to 1D and 3D Nano systems. By controlling their size, thickness, and nanostructure, 2D nanomaterials have brought innovations to various water treatment systems, offering outstanding catalytic, adsorptive, and separation capabilities. These systems include ultrathin graphene membranes, efficient oil adsorbents, rapid visible light photocatalysts, and other intelligent/self-healing structures. ⁽⁷⁾

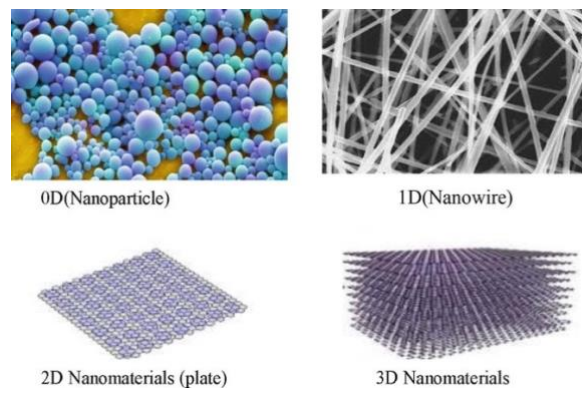


Fig.1 Nanomaterials come in different forms: zero-dimensional (0D), one-dimensional (1D), two-dimensional (2D), and three-dimensional (3D).

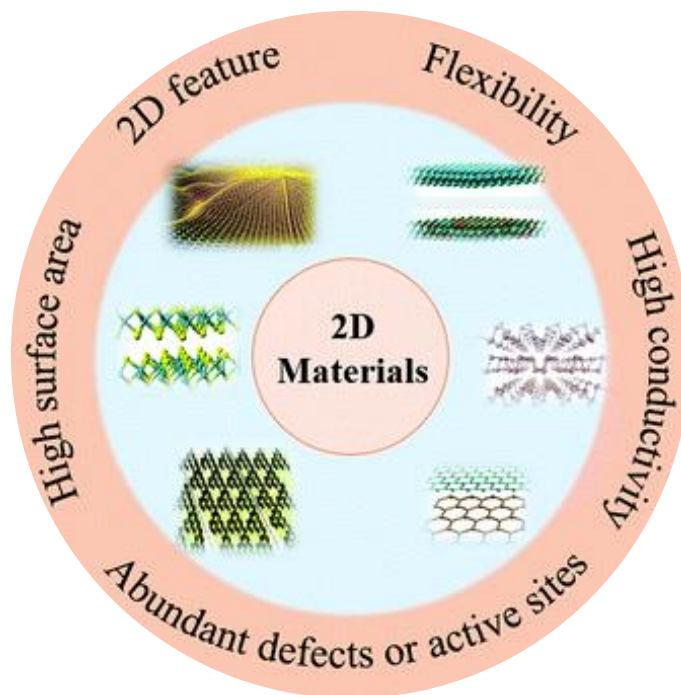


Fig.2 Schematic illustrating the unique properties of 2D materials.

Chapter 2

Pollutants in Water

Water sources have been infiltrated by various contaminants (Fig.3). Compiling an exhaustive inventory of water pollutants proves challenging because pollution comes from many sources, and the diverse origins of pollution depend on factors like location and industrial activities. Nevertheless, below is a compilation of commonly monitored and regulated water pollutants. These pollutants are categorized into different groups:

2.1 Inorganic Pollutants

2.1.1 Heavy Metals

Heavy metals are a class of metallic elements characterized by high density and potential poisonousness, even in small quantities. This category encompasses a range of metals and metalloid substances with an atomic density exceeding 4 g/cm^3 , the same over five times that of water. However, it is crucial to note that the chemical properties of the material are more significant than its density. Heavy metals include the platinum group elements. ⁽⁹⁾ Heavy metals and their detrimental impacts on human health, along with the permissible levels set by the World Health Organization (WHO), are as follows:

- Cadmium (Cd): Associated with kidney damage, osteoporosis, and cancer. WHO acceptable limit: 0.003 mg/L.
- Chromium (Cr): Linked to skin irritation, lung cancer, and liver damage. WHO acceptable limit: 0.05 mg/L.

- Copper (Cu): Excessive levels cause gastrointestinal issues. WHO acceptable limit: 2 mg/L.
- Mercury (Hg): Neurological damage, especially in fetuses. WHO acceptable limit: 0.001 mg/L.
- Lead (Pb): Impacts brain development, cardiovascular health. WHO acceptable limit: 0.01 mg/L.
- Zinc (Zn): High levels cause nausea, vomiting. WHO acceptable limit: 3 mg/L.
- Arsenic (As): Carcinogenic, affects skin, lungs, and bladder. WHO acceptable limit: 0.01 mg/L.
- Nickel (Ni): Linked to lung and nasal cancers. WHO acceptable limit: 0.02 mg/L.

2.1.2 Nutrients

Nutrients are essential for the growth and maintenance of plant and animal tissues in aquatic ecosystems. Small amounts of nitrates and phosphates promote the growth and metabolism of algae, which play a crucial role in the food chain. However, excessive nutrient pollution caused by various human activities such as urbanization, intensive agriculture, recreational activities, population growth, open defecation, and improper waste disposal poses a significant threat to the health of coastal and estuarine ecosystems globally. Fertilizer runoff and unregulated sewage discharges contribute to nutrient levels in specific aquatic environments, leading to pollution in both inland and coastal waters.

(10)

2.1.3 Acids and Bases

Such as sulfuric acid and nitric acid: Acid rain, resulting from pollutants like nitric acid and sulfuric acid, adversely affects both surface waters and groundwaters. It leads to the solubilization of trace metals. The rapid corrosion of metal plumbing in acidic groundwaters poses health risks and increases the costs of potable water. ⁽¹¹⁾ The pH level plays a pivotal role in governing water quality and metal concentrations in aquatic environments, overseeing various chemical processes. Proximity to mining activities exposes water bodies to potential metal pollution and bioaccumulation along the food chain. The impact of acid rain, resulting from nitric and sulfuric acid pollutants, further accentuates metal solubilization in both surface and groundwaters. This is supported by studies revealing acidic groundwaters with low pH values and heightened dissolved aluminum levels. The accelerated

corrosion of metal plumbing in this process poses health risks and escalates costs for potable water. This intricate relationship emphasizes the broader environmental consequences on water quality, with implications for ecosystems, potential effects on human health, and impacts on industrial materials.

(12)

2.2 Organic Pollutants

Organic pollutants seriously harm the water quality, causing problems for fish and other aquatic life by making it hard for them to breathe and disrupting the growth of underwater plants. This not only affects the balance of the ecosystem in the water but also has significant consequences for human health. These pollutants can be categorized into pharmaceuticals, persistent organic pollutants (POPs), personal care products (micropollutants), dyes, pesticides, polychlorinated biphenyls (PCBs), polycyclic aromatic hydrocarbons, and aliphatic hydrocarbons. ⁽¹³⁾

2.2.1 Persistent Organic Pollutants (POPs)

Are organic substances that stick around for a long time, and they're kind of like semi-volatile chemicals. These things are not good – they're toxic and can build up in the environment, water, and even in animals and humans. When they get into the water, they cause harm to the environment, aquatic life, animals, and people. These pollutants mainly come from things like fires in vegetation, volcanic activities, industrial processes, and burning fossil fuels.

2.2.2 Pharmaceuticals

Including antibiotics, anti-inflammatory drugs, and antifungal medications, pose environmental concerns due to their pseudo-persistent and eco-toxic nature. These substances, which accumulate in water through sources like domestic waste and pharmaceutical manufacturing, have adverse effects on both aquatic and human life.

2.2.3 Pesticides

Commonly used in farming, can be divided into organochlorine and organophosphorus types. Organochlorine pesticides, like lindane and DDT, are non-biodegradable and hazardous to both the environment and human health. Organophosphorus pesticides affect the nervous system, non-target tissues, and hormonal balance, causing neurotoxic disorders. These chemicals enter water primarily through agrochemicals.

2.2.4 Polychlorinated Biphenyls PCBs

Are harmful pollutants that come from industrial and chemical waste as well as landfills. They don't break down easily, are toxic, and can cause health issues like immune and reproductive problems, along with neurological disorders.

2.2.5 Polycyclic Aromatic Hydrocarbons (PAHs)

Found in things like toluene and benzene, are pollutants resulting from burning fossil fuels and forest fires. These chemicals are known to be cancer-causing, affecting our immune system and nerves, and posing risks to aquatic life.

2.2.6 Aliphatic Hydrocarbons

Including substances like alkanes and chloroform, come from petroleum products and natural activities. They can harm our central nervous, respiratory, liver, and kidney systems.

2.2.7 Textile Dyes

Textile dyes are chemicals used in the textile industry to give fabrics color and texture. Regrettably, many of these dyes are highly toxic and can even be carcinogenic, posing serious risks to both the environment and human health. Their use has led to various health issues in both animals and humans. Some of these harmful dyes include Chlorotriazine Reactive Red 120 Azo, Disperse Blue 56, Reactive Red 4, Disperse Blue 291, Disperse Red 1, Disperse Orange 1, Alizarin Blue FGRL, Alizarin Red FBL, and others. ⁽¹⁴⁾

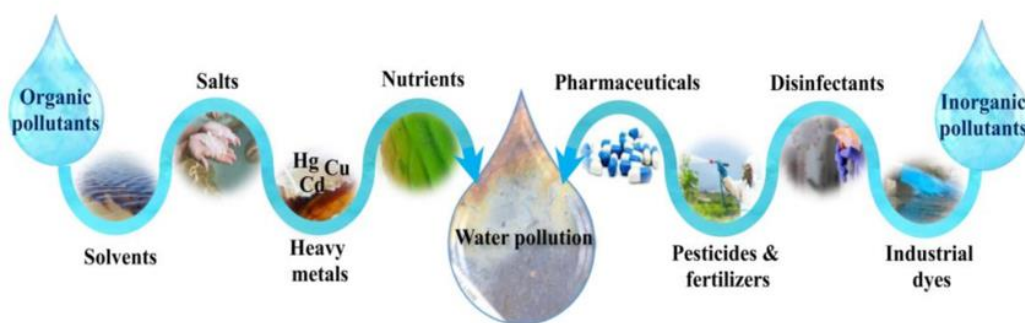


Fig.3 different types of organic and inorganic sources of water pollution

Chapter 3

Two-Dimensional Nanomaterials

In recent years, there has been significant scientific interest in 2D materials due to their unique structure and potential applications. This has led to the creation of a diverse range of 2D-nanomaterials using various methods, accompanied by impressive demonstrations of their practical uses. This chapter will explore some of the most prominent 2D-nanomaterials, including graphene, boron nitride (BN), metal-organic frameworks (MOFs), covalent organic frameworks (COFs), layered double hydroxides (LDHs), molybdenum disulfide (MoS_2), and metal oxides (MXenes), examining their properties relevant to water treatment and methods of preparation.

3.1 Graphene and Graphene oxide

Graphene is like a flat, two-dimensional sheet with a hexagonal pattern, and the carbon atoms within it are tightly connected through covalent bonds. This structure is akin to a chain of polycyclic aromatic

hydrocarbons arranged in a honeycomb crystal lattice, where each repeating unit is made up of two carbon atoms. Graphene functions as a pseudocapacitive material and acts as a fundamental building block for other graphitic allotropes, thanks to its expansive surface area, high conductivity, and commendable mechanical properties. Consequently, graphene emerges as a candidate for enhancing the characteristics of composite materials.

Graphene is a widely used material; however, it exhibits limited thermodynamic stability, with its melting temperature decreasing as thickness decreases. To address this issue, researchers have discovered a solution by oxidizing graphene to produce graphene oxide (GO) or graphene oxide-based composites. GO is the derivate of graphene, which has attracted great attention in environmental pollution treatment.⁽¹⁵⁾ GO features oxygen functionalities on its surfaces and edges, including epoxy, hydroxyl, carboxyl, and carbonyl groups (Fig.4).⁽¹⁶⁾

These modifications result in greater stability, improved solubility in polar solvents, and enhanced compatibility with living organisms. Additionally, the oxygen-related functional components can be easily tailored with various chemical entities, providing versatile applications in areas such as sensing, biomedical fields, and energy storage,⁽¹⁷⁾ and enhance properties such as photocatalysis and adsorption.⁽¹⁸⁾



Fig. 4 structure of graphene and graphene oxide

3.1.1 Synthesis of Graphene and Graphene Oxide

Chemical Vapor Deposition (CVD) stands as a popular technique for the mass production of graphene, offering precise control over its size, quality, and coverage. The process entails heating a substrate, typically copper or other metals, to elevated temperatures, followed by the introduction of a carbon-containing gas like methane. Carbon atoms from the gas then deposit onto the heated substrate, forming a graphene layer. Subsequently, the resulting graphene film can be transferred to alternative substrates as needed (Fig.5). CVD's versatility and ability to tailor graphene properties make it a preferred method for large-scale production in various applications.⁽¹⁹⁾

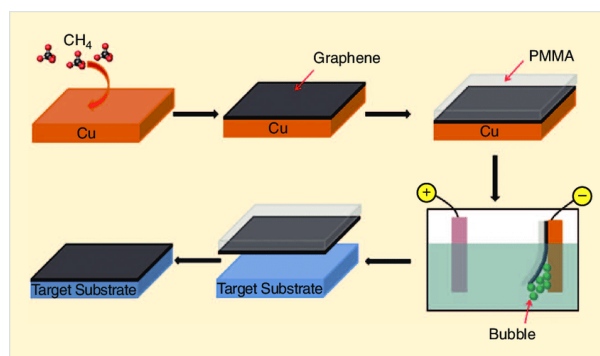


Fig. 5 A schematic of graphene synthesis and the electrochemical transfer process

The most common method for synthesizing graphene oxide is the Hummers method. In 1958, Hummers and Offeman introduced a widely embraced technique for synthesizing graphene oxide (GO). This method begins by combining a specific amount of graphite, sodium nitrate, and concentrated sulfuric acid in a flask chilled to 0°C in an ice-bath. Then, a measured quantity of potassium permanganate is slowly added to the suspension while vigorously stirring. After removing the ice bath, the mixture is heated to 35°C for 30 minutes, followed by an increase to 98°C for 15 minutes. To eliminate residual manganese dioxide and permanganate, 3% hydrogen peroxide is added to the suspension, resulting in colorless, soluble manganese sulfate. The resulting yellowish-brown filter cake undergoes multiple rinses with distilled water before being dispersed in additional distilled water (Fig.6).⁽²⁰⁾

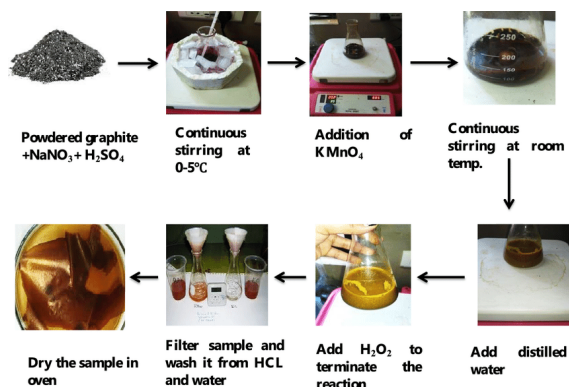


Fig. 6 Synthesis process of graphene oxide with modified Hummer's method

3.1.2 Properties of Graphene and Graphene Oxide

Graphene and graphene oxide offer exceptional properties that make them valuable for water and wastewater treatment. Graphene, with its 2D structure, remarkable mechanical strength, and efficient electrical conductivity, provides a substantial surface area for interactions and remains stable even in harsh chemical environments. Its hydrophilicity further aids in attracting water molecules, enhancing water treatment processes. Graphene Oxide (GO), on the other hand, boasts atomic thickness, oxygen-containing functional groups, and stable laminar structures, making it highly reactive and suitable for various applications, including membranes and adsorbents. Additionally, thin graphene oxide membranes enable ultrafast separation of atomic species, ensuring efficient filtering. These unique characteristics make graphene-based materials crucial for adsorption, membrane technology, and capacitive deionization in water treatment, contributing significantly to effective pollutant removal and sustainable water management. ⁽²¹⁾

3.2 Metal-Organic Frameworks (MOFs)

2D Metal-Organic Frameworks (MOFs) consist of layered structures where extended planes of conjugation are formed by the bonding of metal ions or clusters with organic ligands (Fig.7). ⁽²²⁾ Several linkers in MOFs have been found to be effective in water treatment:

1. Terephthalate (1,4-benzene dicarboxylate or BDC): This is a common linker used in MOFs like UiO-66, which has been studied for its water stability and potential in water treatment. ⁽²³⁾
2. Bipyridyl dicarboxylate (BPYDC): This linker has been used in a core-shell structure MOF (UiO-67-BPY@UiO-66) for water purification. ⁽²⁴⁾

When incorporated into MOFs, these metal ions or linkers can act as catalysts, meaning they can speed up chemical reactions. Because MOFs have lots of tiny pores and a large surface area, they can selectively capture certain molecules. This makes them useful for targeting specific substances in processes like catalysis or capturing pollutants from the water or environment.

The efficiency of a linker in removing contaminants from water can depend on several factors, including the type of contaminant, the specific MOF structure, and the conditions of the water treatment process. ⁽²⁵⁾

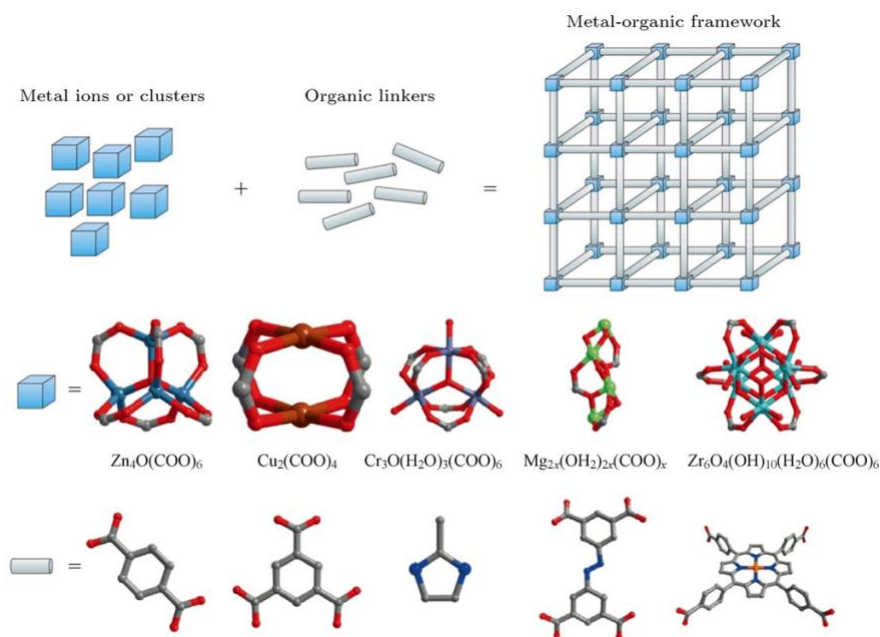


Fig.7 schematic structure of Metal-Organic Frameworks (MOFs), different metal ions and linkers

3.2.1 Synthesis of Metal-Organic Frameworks

The most common method for synthesizing 2D Metal-Organic Frameworks for water treatment is the hydrothermal/solvothermal synthesis method.

Here's a brief overview of the process:

- 1.Preparation: The metal ions and organic linkers are dissolved in a solvent.
- 2.Reaction: The solution is sealed in an autoclave and heated to a specific temperature for a certain period.
- 3.Cooling and Washing: After the reaction, the autoclave is cooled, and the MOFs are collected and washed.
- 4.Activation: MOFs are activated by removing the solvent from the pores, usually by heating under vacuum.

This method can produce MOFs with different compositions, structures, and properties. However, it's worth noting that the choice of metal ions, organic linkers, solvent, temperature, and time can significantly influence the properties of the resulting MOFs. ⁽²⁶⁾

3.2.2 Properties of MOFs

MOFs, as a new kind of porous material, have gained attention due to their customizable pore sizes, exceptional surface area, excellent porosity, and good thermal stability outperforming traditional materials like zeolite and clay. Their unique characteristics have sparked significant interest for applications in areas such as catalytic degradation, separation, adsorption, electrochemical sensors, hydrogen production through catalytic water splitting, and antibacterial engineering. By using MOFs as a starting point, composite materials can be developed by altering metals, substituting organic ligands, or adding functional groups, all with the aim of enhancing the MOF's performance. ⁽²⁷⁾

3.3 Covalent Organic Frameworks (COFs)

Covalent Organic Frameworks (COFs) are a type of crystalline materials, built through covalent bonds from light elements such as carbon, nitrogen, hydrogen, oxygen, and boron. They are constructed entirely from organic building blocks linked by covalent bonds. As a result, many COFs exhibit π -conjugated structures, leading to at least modest electronic conductivity. Moreover, numerous COFs function as organic semiconductors with adjustable band gaps. Additionally, their exclusive covalent connections contribute to high chemical stability. Although the initial COFs lacked water stability, ongoing research has yielded COFs that remain stable even under harsh acidic or basic conditions. ⁽²⁸⁾

3.3.1 Synthesis of COFs

Two-dimensional Covalent Organic Frameworks (2D-COFs) are synthesized by stacking covalently linked COF layers in the vertical direction through weak interaction. The first 2D-COFs, synthesized by condensation reactions of phenyl diboronic acid and hexahydroxytriphenylene(Fig.8). The synthesis process generally involves a high temperature (80–120°C) combined with a low reaction pressure. Almost all COFs, as either bulk materials or thin films grown on the support surface, have been obtained under solvothermal synthesis conditions. This method allows for the precise integration of small organic blocks into an extended, porous framework via covalent linkages. Going beyond bulk 2D-COFs, molecular thin organic layers called COFene can be derived from the exfoliation of 2D-COFs, generating new properties for applications in optoelectronic devices, catalysis, and separation.

⁽²⁹⁾

3.3.2 Properties of COFs

COFs have been proposed as promising materials for water treatment due to their notable intrinsic properties. These properties include excellent chemo stability, high surface area, abundant functional sites, and uniform adjustable aperture size. The unique chemical structural features of COFs promote excellent molecular adsorption from various environments, especially from water. They have been explored for their water remediation ability to a wide range of pollutants including persistent organic pollutants, toxic metals, radioactive wastes, etc. The development of COFs into various microphysical forms such as foams and thick and thin-film membranes has led to a new direction of advanced level water treatment. The notable shift from the granular adsorption of molecular pollutants to rapid and efficient foam-based adsorption and size and chemo-selective membrane-based separation is highlighted.⁽³⁰⁾

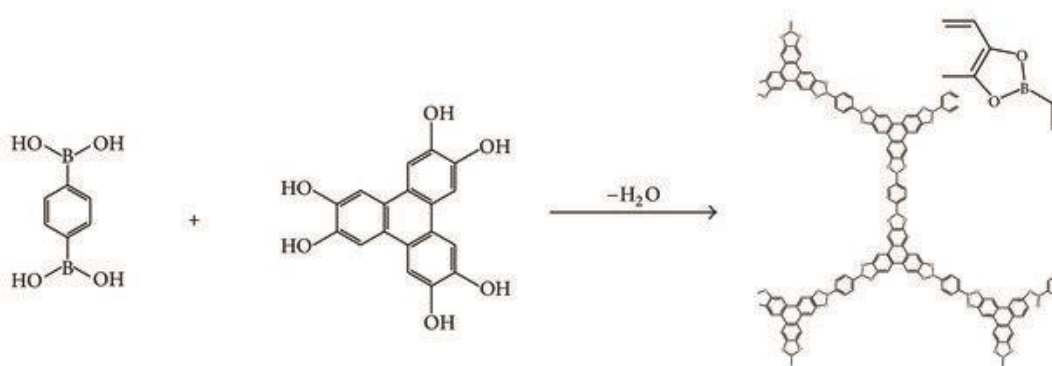


Fig.8 Reaction scheme of phenyl diboronic acid and hexahydroxytriphenylene to produce a 2-dimensional (2D) COFs

3.4 Molybdenum Disulfide (MoS₂)

Molybdenum disulfide (MoS₂) is a type of transition metal dichalcogenide. It possesses a layered structure where molybdenum atoms are chemically linked to two exterior layers of sulfur atoms. Molybdenum disulfide (MoS₂) is a two-dimensional (2D) material that belongs to the family of transition metal dichalcogenides (TMDs). It has a layered structure consisting of individual S–Mo–S units, where the S and Mo atoms are bonded via strong ionic-covalent bonds, and the adjacent layers are held together by weak van der Waals (VDW) forces. MoS₂ can exist in four different crystal phases (Fig.9): a distorted tetragonal phase (1T), hexagonal phases (1H and 2H), and a rhombohedral phase (3R). Among them, 2H-MoS₂ is the most stable and widely found in nature, while 1T-MoS₂ is a metastable state with metallic properties. The crystal phases of MoS₂ have different arrangements of

the S atoms within the S planes, which affect the electronic structures and catalytic activities of MoS₂. The edge sites of MoS₂, where the S atoms are unsaturated, are considered to be the active centers for various reactions, while the basal planes are mostly inert. Therefore, the morphology and phase engineering of MoS₂ are important strategies to enhance its performance in various applications. ⁽³¹⁾

3.4.1 Synthesis of MoS₂

- **Chemical vapor deposition (CVD):** This method involves heating MoO₃ and S powders in a furnace and depositing the MoS₂ vapor on a substrate. This method can produce large-area and high-quality MoS₂ layers with controllable thickness and morphology.
- **Hydrothermal or solvothermal synthesis:** This method involves dissolving Mo and S precursors in a solvent and heating them under high pressure in an autoclave. This method can produce MoS₂ nanosheets or nanoflowers with different phases and sizes.
- **Liquid exfoliation:** This method involves dispersing bulk MoS₂ in a liquid medium and applying ultrasonication or shear forces to peel off the layers. This method can produce MoS₂ nanosheets with tunable thickness and lateral size. ⁽³²⁾

3.4.2 Properties of MoS₂

2D Molybdenum disulfide (MoS₂) exhibits several properties that make it suitable for water treatment applications:

- **High Water Permeability:** The water channels in MoS₂ are smooth, resulting in a 2–10 times faster water passage rate compared to other materials.
- **Stability:** MoS₂ exhibits good stability in a wide range of pH aqueous solutions and mechanical stability under pressure.
- **Biological Compatibility:** Nanopores in MoS₂ membranes have shown enhanced biological compatibility and higher signal-to-noise ratio for biological sensing applications.
- **Desalination:** MoS₂ membranes have been found to be excellent candidates for water desalination.

- **High Surface Area:** MoS₂ has a large surface area, mechanical strength, and tunable surface chemistry, which make it attractive for various applications, including water treatment.
- **Adsorbent or Photocatalyst:** MoS₂ can be used as an adsorbent or a photocatalyst to remove organic and inorganic pollutants from water, such as heavy metals, dyes, drugs, and pesticides. ⁽³³⁾

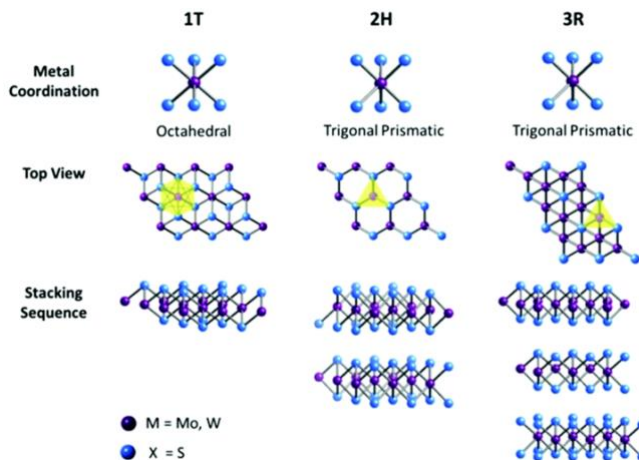


Fig.9 The three structures of MoS₂, 1T, 2H, and 3R, exhibit different coordination and stacking sequences.

3.5 Layered Double Hydroxides (LDHs)

Layered Double Hydroxides (LDHs) can be described by the general formula:

$$[M_{1-x}^{2+} M_x^{3+}(\text{OH})_2]^{x+} [(A_{x/n}^{n-}) \cdot y\text{H}_2\text{O}]^{x-}. \quad (48)$$

In LDHs, brucite-like layers contain a mix of divalent and trivalent metal cations, resulting in a positive charge. The interlayer spaces accommodate exchangeable inorganic or organic anions, connected to the host layers via hydrogen bonds. The tunability of metal cations and charge-compensating anions allows for diverse nanoarchitectures with tailored properties. LDHs find applications in electrocatalysis, photo electrocatalysis, adsorption, and polymer additives. During the oxygen evolution reaction (OER), both M²⁺ and M³⁺ participate in redox reactions, potentially involving electron transfer between them. Anions (Aⁿ⁻) play a role in compensating the positive charge and influencing adsorption/desorption processes within LDHs (Fig.10). ⁽³⁴⁾

3.5.1 Synthesis of LDHs

The synthesis of 2D LDHs can be classified into two main approaches: direct synthesis and chemical exfoliation.

- **Direct Synthesis (Bottom-Up Approach):** Direct synthesis involves building 2D LDH nanosheets from scratch. It's akin to constructing a puzzle piece by piece. In this method, the nanosheets are formed directly through chemical reactions or physical processes. In this technique, short laser pulses are precisely targeted at a solid surface, causing material removal, and facilitating nanosheet growth. The energy from the laser ablates the material, resulting in the formation of thin nanosheets. After that Microwave energy is employed to heat and react materials at an atomic or molecular level. This controlled heating promotes the formation of 2D LDHs. The microwave irradiation method allows for rapid and efficient synthesis. Here, water-in-oil emulsions serve as templates for nanoparticle synthesis. The emulsion droplets act as confined reaction vessels, allowing controlled growth of LDH nanosheets. The reverse microemulsion method provides a route to uniform and well-defined nanosheets.
- **Chemical Exfoliation (Top-Down Approach):** Chemical exfoliation starts with bulk LDH crystals and transforms them into thin nanosheets. It's like peeling layers from an onion. This method involves breaking down the bulk material into smaller units. Initially, layered precursor compounds are prepared. These precursors serve as the starting point for exfoliation. Techniques like coprecipitation, homogeneous precipitation, or topochemical oxidation are used to create these layered structures. Next, ions are inserted between the layers of the precursor. This intercalation process ensures that the layers remain intact but can accommodate additional ions. The intercalated precursor is still a bulk material. Finally, the intercalated compound is dispersed in a liquid or solvent. Through controlled conditions, the layers are separated, resulting in individual nanosheets. The exfoliation process yields thin, flexible sheets with unique properties. ⁽³⁵⁾

3.5.2 Properties of LDHs

LDHs have the following features:

- They consist of stacked layers of mixed metal hydroxides with intercalated anions and water molecules in the interlayer space.
- They have high anion exchange capacity, good thermal stability, and a large specific surface area, which can effectively adsorb and remove heavy metal ions, inorganic anions, organic pollutants, and oil pollutants from wastewater.

- They can be modified by doping, intercalating, or hybridizing with other materials to enhance their adsorption performance and selectivity. ⁽³⁶⁾

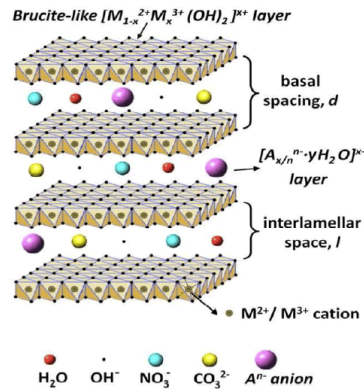


Fig.10 schematic structure of LDHs

3.6 MXenes

MXenes, a diverse family of early transition metal carbides and nitrides, typically follow the formula:

$$M_{n+1}X_nT_x.$$

Here, M denotes early transition metals like Titanium or Chromium, while X represents Carbon or Nitrogen situated at octahedral sites, and T indicates a surface terminal group such as F, -OH, or O. MXenes are primarily produced by removing A element from the precursor MAX phase and introducing T. The MAX phase encompasses ternary carbides or nitrides, with A being an element from group 13 or 14 (e.g., Aluminium or Gallium), stacked alternately with A and $M_{n+1}X_n$ in a multilayered structure. MXenes often exhibit accordion-like shapes but can also form swirl shapes, flower-like porous structures, nanofibers, and nanoribbons via various ultrasonic and processing techniques. ⁽³⁷⁾

3.6.1 Synthesis of MXenes

MXenes synthesis involves two primary steps: the removal of the A component from the MAX phase, and the exfoliation of a 2D sheet (Fig.11). If the resulting structure has fewer than five layers, it is referred to as MXenes. Currently, the main methods for MXenes preparation include pyrolysis, gas phase etching, and chemical liquid phase etching. The pyrolysis method involves decomposing MAX into $M_{n+1}X_n$ under high temperature and vacuum conditions. However, this process also leads to the

sublimation of A and M substances, necessitating the careful selection of the decomposition temperature. The vapor phase etching method employs chlorine gas etching, which is highly corrosive. It is essential to strictly control the etching time and choose an etchant with suitable activity to prevent the etching of the M phase. Chemical liquid phase etching includes several methods such as molten salt, hydrothermal, electrochemical, fluorine-containing acid, and Lewis's acid etching. ⁽³⁸⁾

3.6.2 Properties of MXenes

MXenes are promising materials for water treatment and environmental remediation due to several key properties:

- **Hydrophilicity:** MXenes are readily absorbed or dissolved in water, which makes them suitable for water treatment applications.
- **High Surface Area:** MXenes have a high surface area, which increases their capacity to adsorb pollutants.
- **Activated Metallic Hydroxide Sites:** These sites on MXenes can interact with various pollutants, enhancing the removal efficiency.
- **Nontoxicity:** MXenes are generally non-toxic, making them safe for use in water treatment.
- **Conductive and Flexible:** The unique “conductive clay-like” properties of MXenes allow them to be easily processed by various methods.
- **Tunable Intercalation:** The interlayer spacing in MXenes can be tuned, which can be beneficial for selective ion sieving. ⁽³⁹⁾

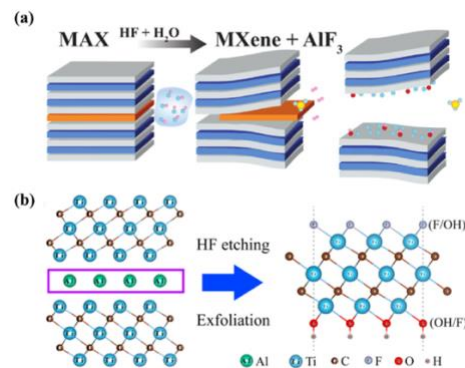


Fig. 11 Schematic diagram of the synthesis of MXenes a) Removal of A Component, b) Exfoliation of 2D Sheet

3.7 Boron Nitride

2D-hexagonal boron nitride (2D-hBN), also known as graphitic boron nitride, exhibits a layered honeycomb structure similar to graphite. Within each monolayer, alternating boron (B) and nitrogen (N) atoms form strong covalent bonds. These layers are held together by weak van der Waals forces (Fig.12). The interlayer spacing in h-BN is approximately 3.3 Å, resembling graphene but smaller than other 2D nanomaterials. Notably, the monolayers follow an ABAB stacking pattern (The ABAB stacking pattern refers to the arrangement of layers in certain crystalline materials, including graphene and hexagonal boron nitride (h-BN)). Overall, 2D-hBN combines stability, adsorption capacity, and ease of separation, making it a promising material for water purification and remediation. ⁽⁴⁰⁾

3.7.1 Synthesis of Boron Nitride

Hexagonal boron nitride (h-BN) is synthesized via the Chemical Vapor Deposition (CVD) technique. The process involves several steps: substrate preparation (cleaning and ensuring a smooth surface), introduction of boron and nitrogen-containing precursor gases into a controlled reaction chamber, dissociation of these gases at elevated temperatures to release boron and nitrogen atoms, surface reaction leading to h-BN layer formation, nucleation on the substrate, precise control of growth parameters (temperature, pressure, and gas flow rates), determination of film thickness by growth rate, and finally, cooling and annealing to enhance crystallinity. CVD enables the controlled growth of high-quality h-BN films, making it valuable for various applications. ⁽⁴¹⁾

3.7.2 Properties of Boron Nitride

Boron nitrides have the following properties that make them useful in water treatment:

- **High Surface Area:** 2D-hBN offers a large specific surface area, providing abundant adsorption sites for pollutants.
- **Bioinert and Stable:** It remains stable under harsh chemical and thermal conditions.
- **Hydrophobic Nature:** 2D-hBN is inherently hydrophobic, allowing easy separation of the adsorbent from contaminated water.
- **Regenerability:** BN adsorbents can be regenerated without damaging the material, making them reusable.
- **Desalination and Dye Rejection:** When incorporated into thin film composite and mixed matrix membranes, 2D-hBN enhances permeance, dye rejection, and desalination. ⁽⁴²⁾

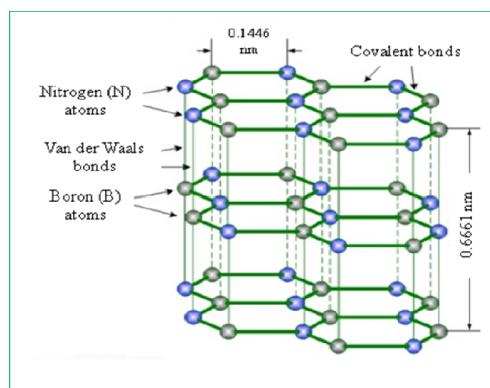


Fig. 12 Schematic of hexagonal boron nitride (h-BN) structure

Chapter 4

Characterization

After synthesizing 2D nanomaterials, it's crucial to characterize them to understand their properties and ensure their quality. Here are some common methods for characterizing 2D nanomaterials:

4.1 XRD

X-ray diffraction (XRD) is a non-destructive technique crucial for characterizing 2D nanomaterials, offering detailed insights into their crystallographic structure, chemical composition, and physical properties. Specifically tailored for nanomaterial analysis, XRD accurately measures atomic spacing, identifies strain states in thin films, and discerns structural details such as grain size and defect structure. By utilizing the principle of X-ray scattering within the crystal lattice, XRD generates diffraction patterns that serve as 'fingerprints' for crystal structures, aiding in material identification and analysis of particle size distribution and defects. The experimental setup involves directing a monochromatic X-ray beam onto the sample, rotating it to different angles, and collecting the scattered X-rays with a detector. Bragg's Law governs the diffraction phenomenon, relating the path difference between scattered X-rays to the X-ray wavelength and interplanar spacing in the crystal lattice. ⁽⁴³⁾

The formula is expressed as:

$$2d\sin(\theta) = n\lambda \text{ Where:}$$

- (d) represents the interplanar spacing (the distance between adjacent crystal planes).
- (θ) is the angle of diffraction (the angle between the incident X-ray beam and the diffracted beam).

- (n) is an integer representing the order of diffraction (usually 1 for the first-order diffraction).
- (λ) denotes the wavelength of the X-rays used in the experiment.

By measuring the angle of diffraction and knowing the X-ray wavelength, scientists can calculate the interplanar spacing and gain insights into the crystal structure of the material. ⁽⁴⁴⁾

Through interpretation of diffraction peaks, XRD provides critical information on crystal structure, lattice parameters, phase composition, and crystallite size, enabling applications in material identification, quantitative analysis, stress/strain analysis, and texture analysis. Overall, XRD plays a pivotal role in advancing nanotechnology applications by elucidating the intricate atomic arrangements of 2D nanomaterials (Fig.13). ⁽⁴³⁾

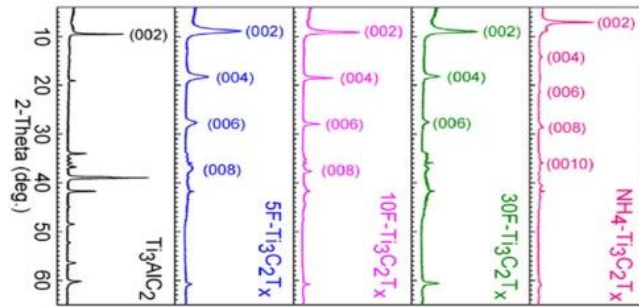


Fig.13 XRD patterns of F-Ti₃C₂T_x and NH₄-Ti₃C₂T_x.

4.2 SEM

Scanning Electron Microscopy (SEM) stands as a pivotal method for characterizing 2D nanomaterials, offering multifaceted insights into their properties. Through high-resolution imaging, SEM unveils the surface morphology, including wrinkles, folds, and defects. Moreover, it enables the examination of layer stacking and edge structures, crucial for materials like graphene. Defect analysis becomes possible, showcasing defects, vacancies, and dislocations, impacting material properties. Furthermore, SEM facilitates simultaneous electromechanical measurements, elucidating conductivity, piezoelectricity, and strain effects. Sample preparation is meticulous, involving steps such as fixation, mounting, coating, drying, and vacuum chamber entry, ensuring accurate imaging and data interpretation. Overall, SEM emerges as a cornerstone in the comprehensive characterization of 2D nanomaterials, offering profound insights into their structure, morphology, and properties (Fig.14).

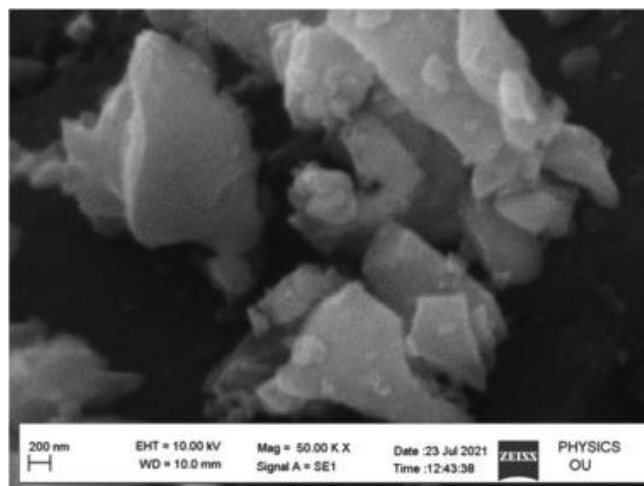


Fig. 14 A picture of graphene oxide in SEM analysis.

4.3 TEM

The Transmission Electron Microscopy (TEM) method is a microscopy-based technique that provides information on the size, morphology, and crystal structure of nanomaterials¹. It's particularly useful for characterizing 2D nanomaterials due to its ability to offer high-resolution images, allowing researchers to observe the atomic structure and identify defects within the materials. TEM operates by transmitting a beam of electrons through a thin specimen and capturing the resulting image, which reflects the sample's structure and composition. This method is essential for understanding the properties of nanomaterials and their potential applications in various fields (Fig.15).⁽⁴³⁾

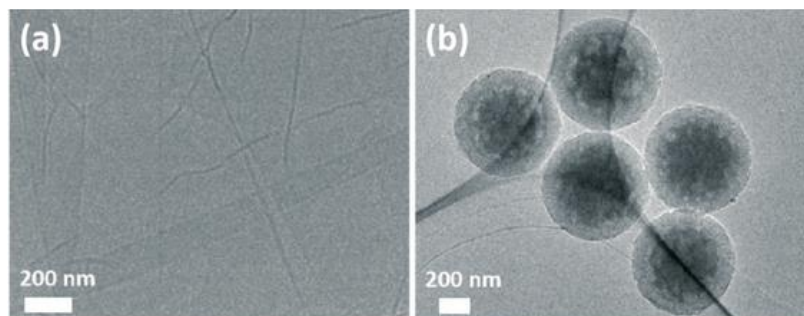


Fig. 15 (a) TEM images of GO and (b)COFs

4.4 FTIR

The FTIR method stands for Fourier Transform Infrared Spectroscopy. It is a technique used for determining the surface composition and ligand binding on nanoparticles. In the context of 2D nanomaterials characterization, FTIR can help identify the types of chemical bonds and functional groups present on the surface of the nanomaterials. This information is crucial for understanding the surface chemistry and interactions of 2D nanomaterials, which can significantly influence their physical properties and potential applications. The FTIR technique operates by passing an infrared light through a sample and measuring the light absorption at different wavelengths. The resulting spectrum represents the molecular fingerprint of the sample, which can be used to deduce the chemical structure. For nanoparticles, this information is vital for tailoring their properties for specific applications (Fig.16).⁽⁴³⁾

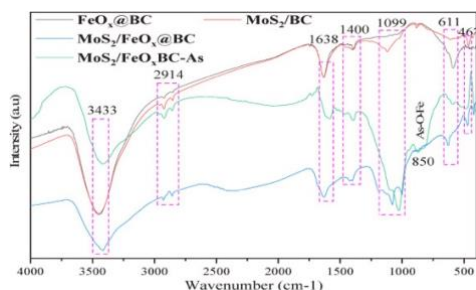


Fig. 16 The FTIR spectra of prepared adsorbents Based on molybdenum disulfide.

4.5 BET

The BET method, which stands for Brunauer-Emmett-Teller method, is a standard technique used to determine the specific surface area of materials. The BET method is utilized in the characterization of 2D nanomaterials to analyze their surface area and porosity. This is crucial for understanding the material's properties and potential applications, especially in fields like catalysis, where surface area plays a significant role in the material's performance. The method involves measuring the amount of gas adsorbed onto the surface of the material and using this information to calculate the surface area. In the context of 2D nanomaterials, the BET method helps in providing insights into their morphological and structural characteristics (Fig.17).⁽⁴⁶⁾

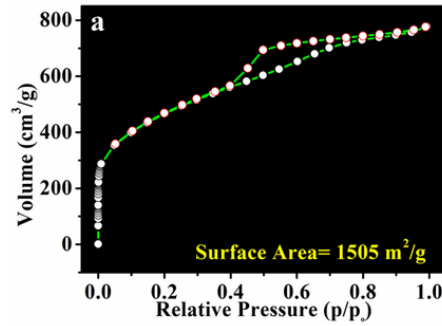


Fig. 17 BET surface area of graphene oxide

4.6 TGA

The Thermogravimetric Analysis (TGA) method is a pivotal technique for monitoring the mass changes of a material under controlled heating. In TGA, the sample is placed on a balance within a furnace, and its mass is meticulously tracked as the temperature rises. The environment around the sample is finely tuned with the introduction of inert or reactive gases, depending on the desired analysis³. The resulting mass fluctuations are captured in thermograms, which are graphical representations of mass loss over time or temperature. TGA is instrumental in detecting transitions such as dehydration or oxidation. For 2D nanomaterials, TGA is invaluable, offering rapid insights into the composition and structure of materials, including nanoparticle coatings and crystallinity (Fig.18).⁽⁴⁷⁾

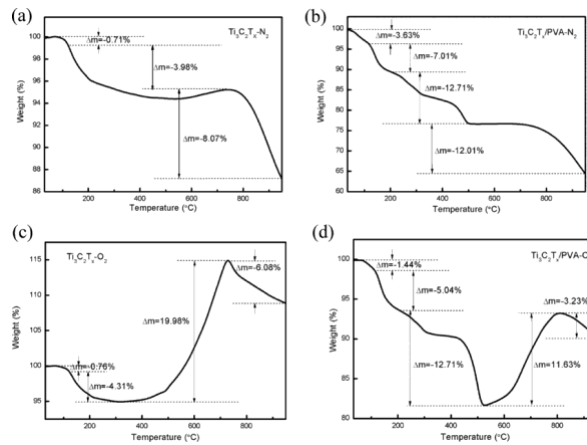


Fig. 18 TG curves of (a) $\text{Ti}_3\text{C}_2\text{T}_x$ and (b) $\text{Ti}_3\text{C}_2\text{T}_x/\text{PVA}$ composites in nitrogen atmosphere and (c) $\text{Ti}_3\text{C}_2\text{T}_x$ and (d) $\text{Ti}_3\text{C}_2\text{T}_x/\text{PVA}$ composites in oxygen atmosphere.

Chapter 5

2D Nanomaterial-Based Water Purification Techniques

2D nanomaterials can use diverse approaches to remove contaminants from water:

5.1 Adsorption

This process involves the adhesion of pollutant molecules onto the surface of the 2D nanomaterial due to physical or chemical interactions. It includes:

- **Strong Interactions:** Nanomaterials provide superior adsorption capabilities owing to the strong interactions that occur between pollutants and adsorption sites, such as π - π stacking and covalent bonds. These interactions enable efficient binding of pollutants to the nanomaterial surfaces, enhancing their removal from the environment.
- **Van der Waals Forces:** The weak van der Waals (vdW) forces present on the surface of 2D nanomaterials enable them to capture pollutants effectively. When pollutants approach the surface of these nanomaterials, temporary fluctuations in electron distribution create an instantaneous dipole in the pollutants. This induced dipole interacts with the 2D nanomaterials' surface through vdW forces, resulting in an attraction that pulls pollutants towards the layers of the nanomaterials.
- **Electrostatic Interactions:** Charged functional groups, whether positive or negative, present on nanomaterials facilitate interactions with oppositely charged pollutants. This enables

nanomaterials to engage in ion exchange processes with pollutants in solution. Through these interactions, nanomaterials effectively remove pollutants by exchanging ions, contributing to efficient purification of the solution.

- **Hydrophobic Interactions:** Hydrophobic pollutants, which are typically repelled by water, are naturally attracted to hydrophobic regions on nanomaterial surfaces. Nanomaterial surfaces often possess hydrophobic patches due to their sp^2 structure. These hydrophobic interactions serve to selectively adsorb organic pollutants, effectively removing them from the surrounding aqueous environment.
- **Hydrogen Bonds:** Functional groups on nanomaterials have the ability to form hydrogen bonds with certain pollutants. This interaction allows for strong binding between the nanomaterial surface and the pollutants, thereby enhancing the adsorption capacity of the nanomaterial. ⁽⁴⁹⁾

5.1.1 Adsorption of Organic and Inorganic Pollutants by Graphene and Graphene Oxide

Soudagar et al. had synthesised GO by Hummer's method and studied the adsorption of MB dye onto nano-GO surface under different conditions. At a dye concentration of 5 ppm, a dose of 10 mg of nano-GO, and a temperature of 30 °C, the maximum dye removal efficiency was seen to be 96.84% after a 15-min period. The experimental data followed the pseudo-second order model and Freundlich isotherm with $q_{\max}$ value around 429.485 mg/g. They also concluded that adsorption capacity decreased with each cycle because some of the adsorbed MB entraps in the structure of the synthesised GO and lowers the removal percentage. The favorable electrostatic attraction is the main interaction between methylene blue and graphene oxide. As graphene oxide has special nano structural properties and a negatively charged surface, the positively charged methylene blue molecules can be easily adsorbed on it. ⁽⁵⁰⁾

In their study, Mehmeti et al. synthesized graphene oxide (GO) by initially oxidizing graphite using a mixture of sulfuric acid (H_2SO_4) and potassium permanganate ($KMnO_4$). This chemical treatment introduced oxygen-containing functional groups onto the graphite surface, leading to the formation of graphite oxide. Subsequently, the resulting graphite oxide underwent ultrasonication, a process involving exposure to high-frequency sound waves (ultrasound). Ultrasonication caused mechanical agitation and exfoliation, effectively separating the graphite oxide layers into individual sheets and resulting in the formation of graphene oxide (GO). Notably, this GO sample exhibited an impressive $q_{\max}$ value of 237.5 mg/g for specific pesticides, including Lindane, a chlorinated pesticide. Further analysis using density functional theory (DFT) calculations and the non-covalent

interaction (NCI) method revealed that the adsorption of Lindane onto graphene oxide primarily occurs due to van der Waals forces between the aromatic rings of Lindane and the carbon atoms of the adsorbents. ⁽⁵¹⁾

5.1.2 Adsorption of Organic and Inorganic Pollutants by MOFs

Huang et al. introduced HSB-W15-NS, a type of 2D MOF, constructed using mixed ligands of hsb-2 (1,2-bis(4'-pyridylmethylamino)-ethane) and 5 Apia (5-aminoisophthate). This novel material exhibits exceptional capabilities in selectively removing Fe^{3+} ions from water, boasting an impressive Fe^{3+} adsorption capacity of up to 250.81 mg/g, with a removal efficiency of 93%. The presence of multiple active moieties within HSB-W15-NS plays a crucial role in facilitating rapid and efficient Fe^{3+} detection and removal. Detailed studies on the detection and adsorption mechanisms were conducted, utilizing kinetic model analysis, Fourier transform infrared spectroscopy, Raman spectrum analysis, density functional theory calculations, and control experiments. This research provides valuable insights for the design and synthesis of 2D-LMOF (Layered Metal-Organic Framework) nanosheet materials capable of both detection and removal functions. ⁽⁵²⁾

Guo et al. explored the utilization of a MOF material, MIL101(Cr)- SO_3H , for the first time in adsorption removal of FQ (Fluoroquinolone) antibiotic pollutants from wastewater. MIL101(Cr)- SO_3H was chosen due to its excellent stability, high porosity, specific surface area, and abundant - SO_3H polar groups within its structure, rendering it an efficient adsorption material for Norfloxacin, Ofloxacin, and Enoxacin in aqueous solutions. The analysis of the adsorption mechanism revealed that electrostatic interaction between FQs and - SO_3H functional groups plays a vital role during the adsorption process. MIL-101(Cr)- SO_3H demonstrated superior performance compared to other reported adsorbents in terms of adsorption capacities, kinetics, and removal efficiency for FQs. It achieved over 90% removal of FQ molecules during the adsorption process, with a final removal efficiency exceeding 99% at adsorption equilibrium. The exceptional removal efficiency and rapid adsorption rate can be attributed to the large pore cavity and pore window sizes of MIL101(Cr)- SO_3H , indicating its promising potential for treating practical contaminated water, particularly those with lower FQ concentrations. ⁽⁵³⁾

5.1.3 Adsorption of Organic and Inorganic Pollutants by COFs

Jiang et al. introduced a novel EDTA-functionalized COF (TpPa-NH₂@EDTA) synthesized through post-modification aimed at capturing heavy-metal ions. The synthesis of TpPa-NH₂@EDTA involved grafting EDTA dianhydride onto TpPa-NH₂. This newly developed material exhibited high selectivity

and removal efficiencies for various competitive heavy-metal ions, including Ag^+ , Pd^{2+} , Fe^{3+} , Cr^{3+} , Cu^{2+} , and Ni^{2+} , achieving removal rates of over 85% within just 5 minutes at pH 3. ⁽⁵⁴⁾

In their study, G. Li et al. demonstrated the impressive adsorption capacities of various COF (Covalent Organic Framework) materials for heavy metal ions. COF-SH exhibited the highest adsorption capacity for Pb^{2+} ions, reaching a value of $q_e = 239 \text{ mg/g}$, showcasing high sensitivity and selectivity towards Pb^{2+} and Cu^{2+} ions compared to other metal cations like Fe^{3+} , Cd^{2+} , Mn^{2+} , and Cr^{6+} . On the other hand, COF-V displayed remarkable selectivity for Pb^{2+} ions with an adsorption capacity of $q_e = 38.24 \text{ mg/g}$. Additionally, COF-SH exhibited a capture capacity of 225.7 mg/g for Cu^{2+} ions at pH 6.5, with both COFs showing equilibrium times based on the pseudo-second-order kinetics. COF-TP and COF-TE were also utilized as absorbents for Pb^{2+} capture, with q_{max} values of 140 mg/g and 185.7 mg/g , respectively, at pH 6.5, and equilibrium times of 25 minutes. Notably, both COFs could be effectively regenerated using 1% HCl, with COF-TP achieving a removal rate of 95.6% and COF-TE reaching 96.5% after ten adsorption-desorption cycles. These findings underscore the potential of COF materials as efficient adsorbents for heavy metal ion removal from aqueous solutions. ⁽⁵⁵⁾

5.1.4 Adsorption of Organic and Inorganic Pollutants by LDHs

In their study, Song et al. introduced a novel adsorbent by modifying MgAl-LDH with Polyethylene glycol (PEG) to efficiently remove heavy metals from wastewater. The primary adsorption mechanisms identified were Precipitation and Complexation, which substantially contributed to the overall adsorption capacity, accounting for 44.2% to 72.12% and 8.99% to 37.89%, respectively. Supplementary mechanisms included Isomorphous Substitution and Electrostatic Attraction, highlighting the multifaceted nature of the adsorption process. This innovative approach shows promise for enhancing the purification of wastewater contaminated with hazardous heavy metals. ⁽⁵⁶⁾

Bahrami et al. (2022) conducted a study focusing on a newly developed Fe/Cr layered double hydroxide (LDH) designed for the removal of Hg^{2+} ions from water solutions. The researchers systematically investigated various parameters affecting the efficiency of Hg^{2+} ion removal and identified optimal conditions: pH 5, a temperature of 25°C , an adsorbent dosage of 20 mg, and a contact time of 120 minutes. The results revealed that mercury ions adhere to the Fe/Cr LDH adsorbent according to the Langmuir adsorption isotherm, with an impressive maximum adsorption capacity of 116 mg/g . Kinetic data were consistent with a pseudo-second order model. ⁽⁵⁶⁾

5.1.5 Adsorption of Organic and Inorganic Pollutants by Molybdenum Disulfide

The study conducted by Liu et al. introduces two-dimensional molybdenum disulfide (2D-MoS₂) as a remarkably effective adsorbent for the removal of lead ions Pb²⁺ from aqueous solutions. It emphasizes the outstanding adsorption capacity of 2D-MoS₂, reaching an impressive 1479 mg/g, surpassing that of traditional adsorbents. This heightened performance is attributed to the expansive sulfur-rich surface area of 2D-MoS₂, which facilitates chemical adsorption through complex formation with Pb²⁺ ions, along with electrostatic adsorption due to the material's negative charge. The adsorption process is well-described by the Freundlich isotherm model and aligns with both pseudo-first order and pseudo-second-order kinetics models, suggesting a multilayer adsorption mechanism. This research underscores the potential of 2D-MoS₂ in environmental cleanup endeavors, particularly for extracting heavy metals from water bodies. ⁽⁵⁷⁾

The article authored by Khan et al. introduces an innovative method for removing mercury from wastewater by synthesizing a molybdenum disulfide/montmorillonite (MoS₂/MMT) composite. This composite demonstrates an exceptional adsorption capacity, surpassing traditional adsorbents by being able to adsorb up to 1836 mg/g of mercury. The successful integration of MoS₂ and MMT was confirmed through various characterization techniques, including Raman spectroscopy, X-ray diffraction (XRD), and Fourier-transform infrared spectroscopy (FTIR). The adsorption kinetics follow the pseudo-first-order model, while the isotherm data conform to the Langmuir model, indicating highly favorable adsorption at temperatures of 25 °C and 35 °C. This breakthrough suggests that the MoS₂/MMT composite holds significant promise as a highly efficient solution for the remediation of mercury-contaminated water. ⁽⁵⁸⁾

5.1.6 Adsorption of Organic and Inorganic Pollutants by MXenes

In their research, Ibrahim et al. investigate the hydrothermal synthesis of two-dimensional MXenes, specifically Ti₃C₂ and Nb₂C, utilizing low toxicity etching agents NaBF₄ and HCl. This method eliminates the need for high-concentration hydrofluoric acid (HF), resulting in MXenes with larger interlayer distances and enhanced specific surface areas. Notably, Ti₃C₂ demonstrates significant adsorption capacity for the cationic dye methylene blue (MB), achieving an adsorption capacity of 24 mg/g adsorbent over 2 hours. However, both Ti₃C₂ and Nb₂C exhibit negligible adsorption for the anionic dye methyl orange (MO). The superior adsorption performance is attributed to the larger specific surface area of MXenes prepared via the hydrothermal method compared to those prepared by traditional HF etching. ⁽⁵⁹⁾

The article authored by K. Li and colleagues introduces an innovative approach to wastewater treatment by developing MXene-based core-shell nanocomposites. Through a layer-by-layer self-assembly method, these composites are designed to enhance the adsorption of dyes, including Safranin T, Methylene Blue, and Neutral Red, from contaminated water sources. The study elucidates that the adsorption mechanism of the composites follows a pseudo-second-order model, indicating their high efficiency and potential for practical application. Remarkably, these composites maintain considerable adsorption capacity even after multiple uses, suggesting their suitability for repeated applications in large-scale water purification systems. This research not only contributes to environmental remediation efforts but also underscores the versatility of MXene materials in addressing ecological challenges. ⁽⁶⁰⁾

5.1.7 Adsorption of Organic and Inorganic Pollutants by Boron Nitride

In their research, Song et al. focus on the elimination of hexavalent chromium Cr^{6+} , a highly hazardous heavy metal ion, utilizing amine-functionalized porous boron nitride (pBN-AS@MBA). The synthesized material demonstrates a remarkable adsorption capacity of 83.78 mg/g, surpassing that of unmodified pBN. The removal mechanism involves both chemisorption, where Cr^{6+} interacts with amine groups on the sorbent, and electrostatic attractions, particularly evident under acidic conditions. This study highlights the potential of amine-functionalized pBN for effectively removing Cr^{6+} in water treatment applications. ⁽⁶¹⁾

In their study, Tewatia et al. introduce a novel composite material comprising boron nitride quantum dots (BNQDs) anchored onto cellulose nanofibers (CNFs) derived from rice straw, designated as BNQD@CNFs. This composite serves a dual function of detecting and removing mercury ions Hg^{2+} from wastewater. The key findings reveal that BNQD@CNFs effectively integrate the fluorescence properties of BNQDs with the fibrous network of CNFs. Tailored for Hg^{2+} detection and adsorption, the composite demonstrates a notable surface area of 35.147 m^2/g , facilitating efficient adsorption. With a quantum yield of 0.45, it ensures sensitive detection capabilities. Importantly, the composite achieves an impressive 96% removal rate of Hg^{2+} at a concentration of 10 mg/L, with a maximum adsorption capacity of 314.5 mg/g. The removal process relies on strong electrostatic interactions and fluorescence quenching, following pseudo-second-order kinetics and Langmuir isotherm models. ⁽⁶²⁾

5.2 Membrane Filtration

2D-nanomaterials can be used to create membranes that filter out pollutants. 2D-nanomaterials exhibit several properties that make them highly useful in membrane filtration for water treatment:

- **Large Surface Area:** 2D-materials, like graphene, have an enormous surface area due to their single-atom thickness. This large surface area allows for efficient adsorption of pollutants and solutes.
- **High Flux:** The nanometer-level thickness of 2D-materials leads to higher flux rates during filtration. Water can flow through these thin membranes more rapidly.
- **Anisotropic Properties:** Unlike 1D or 3D materials, 2D-nanomaterials exhibit highly anisotropic physical and chemical behavior. Their properties can be tuned to suit specific filtration needs.
- **Tailorable Properties:** 2D-materials offer a vast array of tunable properties. We can adjust their composition, size, and surface chemistry for optimal filtration performance.
- **Chemical Stability:** Many 2D-nanomaterials, such as hexagonal boron nitride (BN), are chemically inert and stable even under harsh conditions, ensuring prolonged membrane durability.
- **Hydrophobic Nature:** 2D-materials are inherently hydrophobic. Hydrophobic membranes can effectively repel water while allowing pollutant adsorption.
- **High Permeance:** When incorporated into membrane architectures, 2D-materials can achieve high permeance. Water flows through these membranes efficiently.
- **Dye Rejection and Desalination:** BN-based membranes exhibit high dye rejection. They are also effective for desalination processes.
- **Enhanced Performance:** By integrating 2D-nanomaterials, we can overcome current membrane shortcomings. These materials significantly enhance the overall performance of water treatment membranes. ⁽⁶³⁾

5.2.1 Graphene and Graphene Oxide-Based Membranes

A study by Hu et al. reported the fabrication and performance of a novel membrane based on Torlon hollow fiber modified by layer-by-layer (LbL) graphene oxide (GO) framework. The membrane showed high rejection of metal ions such as Pb^{2+} , Ni^{2+} and Zn^{2+} under a pressure of 3 bar and a concentration of 1000 ppm. The rejection rates were 95.88%, 99.74% and 98.07% respectively, while the pure water permeability (PWP) was 4.7 LMH/bar. The LbL GO framework enhanced the mechanical strength, hydrophilicity, and antifouling properties of the membrane.

- Carboxylate Interaction: GO nanosheets possess negatively charged carboxylate groups capable of attracting and retaining positively charged metal ions like Mg^{2+} and Cs^+ through electrostatic interactions.
- Size-Exclusion Effect: The interlayer spacing between GO nanosheets, approximately 1 nm, is smaller than the hydrated radius of most metal ions. This size discrepancy results in a size-exclusion effect, preventing the entry of metal ions into the interlayer spaces. ⁽⁶⁴⁾

Yu et al. developed a double-crosslinked composite graphene oxide nanofiltration membrane (Ca/GO-SAx) for the effective separation of dyes from textile wastewater. The membrane demonstrated outstanding performance in removing methylene blue, Congo red, crystal violet, and direct red 80 dyes, with each dye being removed by more than 98.80%. The mechanism underlying dye separation was attributed to the molecular sieve effect of the nanochannels within the membrane and the electrostatic repulsion between the membrane surface and the dye molecules. ⁽⁶⁵⁾

5.2.2 MOFs-Based Membranes

Zhu et al. fabricated ZIF-8 (Zeolitic imidazolate frameworks (ZIF-8) are a class of metal-organic frameworks (MOFs)) by adding PSS (poly(sodium 4-styrenesulfonate)) and ZIF-8 in a solution and fabricated a TFN-ZIF membrane over a layer of polyamide that made a uniform membrane with more hydrophobicity and also increased the original permeability by two folds. ZIF-8 is used for the elimination of K^+ , Ca^{2+} , Cl^- , Mg^{2+} , Sr^{2+} , Br^- , SO_4^{2-} by size exclusion mechanism with about 99 % rejection and flux of 13.5 kg/m².

- During the passage of an ion-containing solution through the membrane, ZIF-8 selectively interacts with particular ions.
- The pores of the membrane permit smaller water molecules to permeate while blocking larger ions. ⁽⁶⁶⁾

Zhang and his colleagues used UiO-66- $(\text{COOH})_2$ for separation of organic dyes using electrostatic interaction. The high rejection of UiO-66- $(\text{COOH})_2$ /prGO (reduction graphene oxide/metal-organic frameworks nanoscale laminated membrane) ($98.2 \pm 1.7\%$ for negatively charged Congo red and $92.55 \pm 2.5\%$ for positively charged methylene blue) were exhibited. Moreover, the rejection for heavy metal ions also can be efficiently improved up to $96.5 \pm 83.1\%$ for Cu^{2+} and $92.6 \pm 80.4\%$ for Cd^{2+} , indicating the positive effect of the electrostatic interaction on the nanochannels for ions. ⁽⁶⁷⁾

5.2.3 COFs-Based Membranes

In their pioneering research, Li et al. synthesized an extraordinary 2D-BTCA-TAPB-COF membrane, composed of benzene-1,3,5-tricarbaldehyde and 1,3,5-tris(4-aminophenyl) benzene. This membrane consists of nanometer-thick BTCA-TAPB-COF lamellas stacked on porous ceramics, featuring a positively charged surface across a broad pH range. Its primary application lies in efficient desalination, showcasing nearly complete NaCl rejections and high fluxes during processing seawater-level NaCl solutions. Particularly noteworthy is the membrane's exceptional stability for desalination, achieving close to 99.9% NaCl rejection through pervaporation, surpassing numerous polymeric membranes. ⁽⁶⁸⁾

In their recent work, Li et al. developed a composite material named MF@COF, tailored for environmental protection with a specific focus on ultrafast removal and on-site quick assessment of Cd^{2+} pollution. This composite is created through the in-situ growth of an N/O-rich COF (Covalent Organic Framework) on the surface of a melamine foam (MF), merging the macro-porous channels of MF with the crystallinity of COF. The primary objective of this integration is the removal of heavy metal ions, particularly Cd^{2+} (Cadmium ions), although it shows promise for capturing various other heavy metal ions as well. The material demonstrates an impressive maximum adsorption capacity for Cd^{2+} of 278.45 mg/g, with adsorption equilibrium achieved within 1–3 seconds. Kinetic analysis reveals that the adsorption kinetics adhere to a pseudo-second-order model, while the adsorption isotherm conforms to the Freundlich model, indicating rapid and efficient capture capability. ⁽⁶⁹⁾

5.2.4 LDHs-Based Membranes

In their research, Ghiasi et al. focused on nanocomposite polyvinyl chloride (PVC) hollow fiber membranes incorporated with bentonite and layered double hydroxide (LDH) nanoclays, serving as both natural and synthetic adsorbents to enhance boron removal efficiency. Efficient removal of boron is pivotal for desalination plants, given its prevalence in seawater and potential harm at high concentrations. The study contributes significantly to advancing membrane technology for water treatment and desalination purposes. Notably, membranes containing LDH exhibited superior performance, achieving over 83.6% boron removal and a water flux of 16.1 L/m².h at an operational pressure of 4 bar, surpassing the performance of membranes containing bentonite. ⁽⁷⁰⁾

In their study, Usmani et al. explore the efficient removal of hexavalent chromium Cr^{6+} from water utilizing a composite material composed of magnesium-iron layered double hydroxide supported on orange peel (Mg-Fe LDH@OPP). Compared to raw orange peel powder (OPP), Mg-Fe LDH@OPP

demonstrated superior Cr^{6+} sorption from aqueous media, achieving complete removal under optimized conditions. The highest removal efficiencies were observed at a pH of 2, an adsorbent dosage of 2 g/L, a contact time of 180 minutes, and a temperature of 25°C for a solution with an initial Cr^{6+} concentration of 20 mg/L. The study indicates that complexation reactions and reduction pathways play significant roles in Cr^{6+} removal using Mg-Fe LDH@OPP, whereas ligand exchange is crucial for OPP. Moreover, Mg-Fe LDH@OPP exhibited greater applicability than raw OPP, with prolonged breakthrough and exhaustion times, suggesting its potential as a promising material for treating polluted water. ⁽⁷¹⁾

5.2.5 Molybdenum Disulfide-Based Membranes

In their study, Tian et al. explore the integration of two-dimensional molybdenum disulfide oxide (O-MoS₂) to enhance tight ultrafiltration (TUF) membranes. The optimized O-MoS₂/PES membrane exhibits impressive rejection rates for small molecules such as PEG 10 kDa (92.67 ± 0.12%) and Rose Bengal (99.9%), highlighting its effectiveness in separating dyes and natural organic matter. Through the incorporation of 2.0 wt% O-MoS₂, the membrane's molecular weight cut-off (MWCO) is significantly reduced from 15322 Da to 8404 Da, enhancing selectivity. Furthermore, the membrane demonstrates a high pure water flux of 75.24 ± 4.29 L/m².h.bar. These enhancements are attributed to the O-MoS₂ nanosheets, which adjust pore sizes, improve hydrophilicity, and mitigate fouling, marking a promising advancement in water purification technology. ⁽⁷²⁾

The study conducted by Wang et al. represents a significant breakthrough in water treatment technology with the development of thin-film nanocomposite (TFN) nanofiltration membranes incorporating carboxyl group-grafted molybdenum disulfide (COOH-MoS₂) nanoparticles. Synthesized through an organic functionalization grafting process, these nanoparticles play a crucial role in enhancing membrane performance. The COOH-MoS₂ modified membranes exhibit impressive pollutant removal capabilities, achieving over 98.5% rejection for Na₂SO₄ while maintaining a low NaCl rejection of 23.8%. Notably, the optimal TFN membrane demonstrates a water permeance of 27.7 LMH/bar, a significant improvement compared to both the control membrane's 9.6 LMH/bar and the original MoS₂ modified membrane's 18.4 LMH/bar. This enhancement is primarily attributed to the increased hydrophilicity of the nanoparticles, effectively restricting piperazine monomer diffusion and resulting in the formation of a thinner and more loosely structured selective layer. Such innovation not only enhances water filtration efficiency but also offers a promising solution to address global water scarcity challenges. ⁽⁷³⁾

5.2.6 MXene-Based Membranes

Sun et al. present a comprehensive examination of MXene-based membranes, highlighting their potential in addressing the global water scarcity challenge. The study delves into the unique properties of $\text{Ti}_3\text{C}_2\text{T}_x$, the most extensively researched MXene, which exhibits exceptional chemical, thermal, mechanical, and electronic characteristics, rendering it an ideal candidate for fabricating water treatment membranes. These membranes have demonstrated remarkable proficiency in purifying water by effectively removing a plethora of pollutants, including organic dyes, antibiotics, radionuclides, and heavy metals such as Th^{4+} , U^{6+} , Ba^{2+} , Sr^{2+} , Cu^{2+} , Hg^{2+} , and Pb^{2+} . Notably, the adsorption capacity of MXene for Sr^{2+} and Ba^{2+} is impressive, achieving equilibrium within an hour and showcasing a rapid adsorption rate. The underlying mechanisms facilitating this removal process encompass ion exchange, the formation of inner-sphere complexes, and electrostatic attraction. Furthermore, the integration of MXene with ultrafiltration systems has been shown to enhance dye retention, particularly at elevated pH levels, owing to the abundance of negative functional groups on MXene. ⁽⁷⁴⁾

The study conducted by Ding et al. introduces a ground-breaking lamellar membrane constructed from two-dimensional $\text{Ti}_3\text{C}_2\text{T}_x$ MXene nanosheets, showcasing remarkable efficiency in water purification. This membrane exhibits selective rejection of molecules larger than 2.5 nm, including pollutants such as Evans blue and Cytochrome c, as well as gold nanoparticles. Its exceptional water permeance, exceeding 1000 L/m². h. bar, significantly surpasses that of comparable membranes, marking a notable advancement in the field. The superior performance of the membrane is attributed to the short transport pathways and abundant nanochannels provided by the MXene nanosheets, achieved through a meticulous preparation process. Beginning with Ti_3AlC_2 , the material undergoes HF etching to produce $\text{Ti}_3\text{C}_2\text{T}_x$, which is then exfoliated via sonication and carefully assembled on an anodic aluminum oxide substrate. This innovative approach yields a membrane characterized by not only high permeance but also outstanding stability and rejection rates, thus offering promising prospects for more effective water purification solutions. ⁽⁷⁵⁾

5.2.7 Boron Nitride-Based Membranes

The study by Daneshnia et al. presents an innovative approach to water purification by integrating Cyclopentadienyl-functionalized Boron Nitride Nanosheets (CBNs) into thin film nanocomposite (TFN) membranes. These membranes demonstrate a remarkable 95% efficiency in removing sodium sulfate (Na_2SO_4), significantly enhancing water flux by 22.10% over traditional membranes. This leap in performance is primarily due to the augmented hydrophilicity and surface roughness provided by the CBNs, which facilitate a stronger interaction between water molecules and the membrane surface,

thus improving the membrane's water permeability and antifouling properties. Additionally, the TFN membranes exhibit robust antibacterial capabilities against *Escherichia coli*, making them highly effective for water treatment applications. The integration of CBNs not only optimizes the membrane's filtration capacity but also contributes to its mechanical and thermal stability, positioning it as a promising solution for addressing global water scarcity challenges. ⁽⁷⁶⁾

The study conducted by Lee et al. introduces an innovative approach to semiconductor wastewater treatment by developing functionalized boron nitride (BN) ceramic nanofiltration membranes. Through the utilization of two distinct functionalization techniques—strong acid oxidation and tannic acid (TA)-assisted exfoliation—the researchers successfully introduced hydroxyl groups onto BN surfaces. This advancement resulted in the creation of ceramic nanofiltration (NF) membranes, which, when applied to ceramic ultrafiltration (UF) membrane substrates, exhibited a significant enhancement in performance. The membranes demonstrated a notable increase in the rejection rates for dissolved silica and humic acid—20.4% and 59.8%, respectively—compared to the ceramic UF membrane alone. This superior separation capability is attributed to the altered surface chemistry and the integration of nanochannels within the ceramic membranes, facilitated by the BN nanomaterials. These findings underscore the potential of BN-functionalized ceramic NF membranes in achieving more efficient and effective wastewater treatment in the semiconductor industry. ⁽⁷⁷⁾

5.3 Photocatalysis

2D nanomaterials can act as photocatalysts, absorbing light and using this energy to break down pollutants. When exposed to light, they generate reactive species that degrade organic and inorganic pollutants. These materials can be immobilized on surfaces or incorporated into coatings.

The photocatalytic degradation mechanism involves several sequential steps:

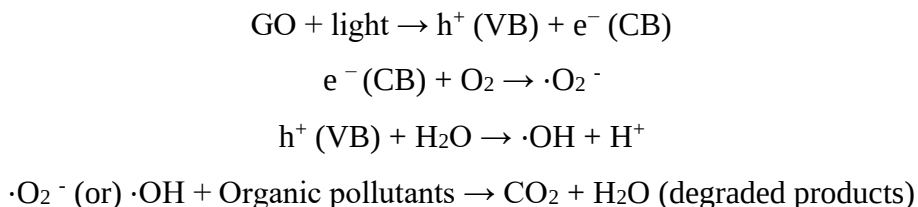
- **Generation of Electron-Hole Pairs:** When the photocatalyst absorbs photons with sufficient energy, electron-hole pairs are generated. This process occurs in response to the absorption of light wavelengths by the material.
- **Separation of Electron-Hole Pairs:** Upon excitation, electrons are promoted from the valence band (HOMO) to the conduction band (LUMO), creating free electrons and positively charged holes. This separation of charges is a crucial step in the photocatalytic process.

- **Transfer of Charges to Catalyst Surface:** The generated electrons and holes migrate to the surface of the photocatalyst material. Here, they can participate in surface reactions with adsorbed species.
- **Redox Reactions:** Once on the surface, the electrons and holes facilitate redox reactions with adsorbed species, such as organic pollutants or oxygen molecules. Electrons can reduce these species, while holes can oxidize them, leading to the degradation of pollutants into harmless byproducts. ⁽⁷⁸⁾

5.3.1 Graphene and Graphene Oxide as A Photocatalyst to Remove Organic and Inorganic Pollutants.

When Graphene Oxide (GO) is exposed to light, it absorbs photons, which excite electrons from the valence band (VB) to the conduction band (CB), creating electron-hole pairs. The excited electrons (e^-) in the conduction band (CB) react with oxygen molecules (O_2) to form superoxide radical anions ($\cdot O_2^-$). The positive holes (h^+) in the valence band react with water molecules (H_2O) to produce hydroxyl radicals ($\cdot OH$) and hydrogen ions (H^+). The superoxide radical anions or hydroxyl radicals then react with organic pollutants, leading to their degradation into carbon dioxide (CO_2) and water, which are less harmful products.

Stepwise degradation of pollutants by GO is given as:



Wang et al. synthesized GO using a process involving treatment of graphene flakes with $NaNO_3$ and H_2SO_4 , followed by oxidation with $KMnO_4$. The synthesized GO exhibited photocatalytic activity for the degradation of various aromatic micro-pollutants (AMPs). The study demonstrated successful degradation of AMPs within 60 minutes, with photodegradation efficiencies ranging from 91.68% to 31.28%, depending on the specific molecular structural characteristics of the AMPs. ⁽⁷⁹⁾

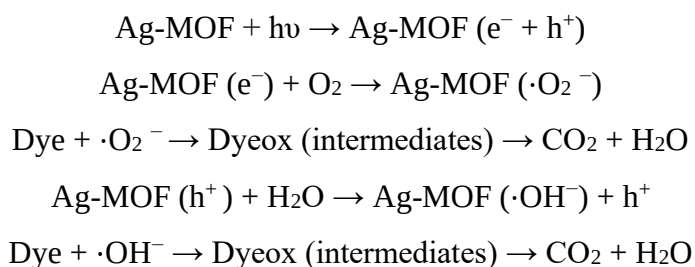
Krishnamoorthy et al. utilized graphite powder treated with H_2SO_4 and $KMnO_4$ to prepare GO nanosheets with UV-active properties. These GO nanosheets showed efficient degradation of Methyl orange (MO) dye in the presence of electron scavengers such as peroxymonosulfate (PMS). The study revealed that GO exhibited a degradation efficiency of 91% towards MO dye in the presence of PMS.

Additionally, the photocatalytic degradation rate of Methylene blue (MB) dye by different concentrations of GO nanosheets in the presence of electron scavengers was investigated, showing promising results. ⁽⁸⁰⁾

5.3.2 MOFs as A Photocatalyst to Remove Organic and Inorganic Pollutants

Within metal-organic frameworks (MOFs), three distinct sites can be harnessed for photocatalytic processes: metal clusters, organic ligands, and internal cavities. Organic ligands possess the ability to capture light energy, initiating the generation of photogenerated charges that are subsequently transferred to metal sites. This transfer mechanism is facilitated through either linker-to-cluster charge transfer (LCCT) or linker-to-metal charge transfer (LMCT). Similarly, metal clusters within MOFs can function as discrete semiconductor quantum dots, absorbing light energy and transferring the resulting photogenerated charge to organic ligands via metal-to-linker charge transfer (MLCT). Furthermore, the internal cavities present in MOFs can be infused with guest photoreactive materials, such as metal nanoparticles (NPs) or semiconductors, thereby enhancing their photocatalytic capabilities. ⁽⁸¹⁾

Kitchamsetti et al. synthesize Ag-MOF nanosheets and then applied them as a photocatalyst to remove different organic pollutants they defined the removal of organic dye pollutants by photocatalytic mechanism as follows:



(e represents electron, $h\nu$ light, h hole, $\cdot\text{O}_2^-$ superoxide radicals, and $\cdot\text{OH}^-$ hydroxyl radicals)

The Ag-MOF nanosheets displayed remarkable performance of photocatalytic activity for the removal of under the illumination of a Xenon lamp. Dye removal percentages of 74.5, 85.5, and 90.7% for MO, CV, and MB dyes were obtained for the optimized photocatalytic activity. ⁽⁸²⁾

Kim et al. conducted a study where they synthesized a Zr-based metal-organic framework (MOF) using pyrene and porphyrin building blocks, resulting in a nano-sized material referred to as nano-

sized mixed ligand MOF (nMLM). This nMLM was employed for the degradation of Rhodamine B (Rh-B) in the presence of H₂O₂. The nanoscale MOF (n-MOF), with its diverse catalytic active sites, exhibited remarkable efficiency by completely degrading Rh-B within 240 minutes.

- **Energy Transfer:** The nMLM utilizes energy transfer from pyrene to porphyrin ligands within its structure, thereby enhancing its light-harvesting capabilities.
- **Electron Transfer:** Subsequent electron transfer from the porphyrin to the Zr-oxo cluster prevents electron-hole recombination, thereby improving the photocatalytic efficiency.
- **Stability and Recyclability:** The nMLM maintains its structural integrity and photocatalytic performance even after repeated use, demonstrating its robustness and potential for practical applications. ⁽⁸³⁾

5.3.3 COFs as A Photocatalyst to Remove Organic and Inorganic Pollutants

Y. Zhang et al. synthesized a photocatalyst membrane composed of a BiOBr/TzDa COF heterojunction, specifically designed for wastewater purification. This innovative material exhibits efficacy in removing two primary types of pollutants:

- **Organic Dyes:** Notably, Rhodamine B (RhB) can be efficiently degraded by the membrane.
- **Heavy Metal Ions:** The membrane demonstrates the capability to reduce hexavalent chromium Cr⁶⁺ to trivalent chromium Cr³⁺, a less toxic form that can be precipitated for subsequent removal.

The membrane's efficiency is underscored by its ability to remove 97% of both RhB and Cr⁶⁺ from a binary mixture solution within 20 and 40 minutes, respectively, under simulated visible light conditions. This remarkable performance is attributed to the enhanced performance of the Z-scheme heterojunction structure of the membrane, which facilitates accelerated separation and transport of charge carriers, increases specific surface area, and enhances visible light absorption. Furthermore, the membrane exhibits notable stability and recyclability, further enhancing its potential for practical application in wastewater treatment processes. ⁽⁸⁴⁾

The study conducted by Wu et al. introduces the synthesis of a porphyrin-based covalent organic framework (Por-PD-COF), designed to serve as both a selective adsorbent and an efficient photocatalyst. This innovative material exhibits a remarkable capacity to selectively adsorb methylene blue (MB) from aqueous solutions containing a mixture of organic dyes, while displaying minimal affinity for methyl orange (MO) and rhodamine B (RhB). The Por-PD-COF demonstrates a high

adsorption capacity, capable of capturing 328.57 mg/g of MB, owing to its expansive surface area, abundant active sites, and stable structure. Additionally, the Por-PD-COF showcases exceptional photocatalytic performance, with 99% degradation of MB achieved within 180 minutes under visible light irradiation. Notably, the material exhibits recyclability across multiple cycles without significant loss of adsorptive or photocatalytic efficiency, highlighting its potential as a sustainable solution for the selective separation of specific organic molecules and the removal of organic waste from water.

(85)

5.3.4 LDHs as A Photocatalyst to Remove Organic and Inorganic Pollutants

In their recent study, Sun and colleagues explore a novel photocatalyst comprising Pd-doped SnS nanoparticles adorned with MgAl-layered double hydroxides (LDHs). This innovative material demonstrates remarkable efficiency in eliminating dye pollutants and Cr^{6+} from water. Specifically, the photocatalyst targets the degradation of aqueous rhodamine B (a dye) and the reduction of Cr^{6+} . Under visible light exposure, the Pd-SnS/LDH heterojunctions achieve an impressive 99% degradation performance within just 40 minutes. The heightened photocatalytic activity is ascribed to the prolonged lifetime of photo-induced electrons and efficient interfacial charge carrier transfer, facilitated by robust interactions between Pd-SnS nanoparticles and LDH nanosheets. (86)

The study by Ziwei Wang and colleagues presents an innovative photocatalytic approach for water treatment, introducing a composite catalyst, LDH@LFO, that synergistically harnesses layered double hydroxides and lanthanum ferrite to activate peroxymonosulfate. This catalyst stands out for its remarkable efficiency in degrading azo dye acid red 27, achieving a significant 93% reduction within a mere 20 minutes, markedly outperforming traditional photocatalysis or persulfate oxidation methods. The LDH@LFO catalyst's superior performance is attributed to the formation of a p-n heterojunction, which not only facilitates enhanced charge carrier separation but also broadens the range of visible light absorption, thereby accelerating the degradation process and offering a promising solution for mitigating environmental pollution caused by dye wastewater. (87)

5.3.5 Molybdenum Disulfide as A Photocatalyst to Remove Organic and Inorganic Pollutants

The study by Li et al. introduces an innovative Fe-MoS₂ photocatalyst, synthesized via a hydrothermal method, showcasing exceptional performance in water decontamination. This catalyst effectively activates peroxymonosulfate to degrade tetracycline hydrochloride in water, achieving an impressive 92% degradation efficiency under visible-light irradiation. Its distinctive dual metallic active sites, comprising iron and molybdenum atoms, not only amplify the production of photoelectrons from

MoS₂ but also facilitate the regeneration of Fe²⁺, ensuring minimal iron leakage and superior recyclability. This advancement in photocatalyst design holds significant promise for enhancing water purification processes. ⁽⁸⁸⁾

In their study, Yuan et al. delve into the synthesis and photocatalytic performance of few-layer MoS₂/graphene hybrids. These hybrids are created through a hydrothermal method, resulting in MoS₂ nanoflakes grown on graphene surfaces. Notably, the photocatalytic experiments reveal that these MoS₂/RGO (Reduced Graphene Oxide) hybrids effectively decompose methylene blue (MB), a common pollutant, when exposed to both UV and visible light. Impressively, under UV light, the hybrids achieve complete MB decomposition within 55 minutes, while under visible light, it takes just 75 minutes—outperforming even the commercial P25 photocatalyst (nano TiO₂ powder), particularly in visible light conditions. The enhanced photocatalytic performance is attributed to the synergistic effect between the few-layer MoS₂ and graphene, which enhances adsorption and conductivity, leading to improved charge transfer and reduced recombination of photoelectrons and holes. ⁽⁸⁹⁾

5.3.6 MXenes as A Photocatalyst to Remove Organic and Inorganic Pollutants

Wang et al. introduce a novel approach utilizing TiO₂-enriched MXene microfibers as efficient and recyclable photocatalysts for wastewater treatment. Specifically, the focus is on Ti₃C₂T_x, two-dimensional transition metal carbide, nitride, or carbonitride. These photocatalysts effectively target organic dyes in wastewater, particularly Rhodamine B (RhB) dyes. Under optimal calcination conditions (300°C for 3 hours), the TiO₂@Ti₃C₂T_x fibers achieve an impressive 97% degradation of RhB within 60 minutes. The process involves an initial alkalization/de-alkalization pre-treatment of the Ti₃C₂T_x sediment, followed by wet spinning and calcination to enhance the photocatalytic performance. ⁽⁹⁰⁾

Tan et al. investigated a novel photocatalyst called alk-MXene-TiO₂/α-Fe₂O₃-T (MTFX), which exhibits remarkable efficiency in treating pollutants in wastewater. Notable findings include:

- Dye Degradation: MTFX achieves over 90% efficiency in degrading most dyes.
- Antibiotics: It effectively treats antibiotics such as TC, SMZ, and CIP, with over 70% efficiency.
- Metal Ion Reduction: MTFX demonstrates reduction performance for the metal ion Cr⁶⁺.

- Type-II Heterojunction: The MTFX type-II heterojunction, featuring Ti_3C_2 MXene as a co-catalyst, is synthesized via calcination. This design enhances photocatalytic activity by efficiently separating electrons and holes.

- Stability: Even after 7 cycles, the photocatalyst maintains a degradation rate above 70% for Rhodamine B.

These findings highlight MTFX's potential for industrial wastewater treatment due to its high efficiency and stability. ⁽⁹¹⁾

5.3.7 Boron Nitride as A Photocatalyst to Remove Organic and Inorganic Pollutants

In their study, Guo and colleagues introduce a novel floating photocatalyst called BN-DS-7, synthesized from boron nitride (BN) and dredged sediment (DS). The preparation involves calcination of a BN and DS mixture with a mass ratio of 3:7 at 1100°C . BN-DS-7 is specifically designed for photodegrading Neutral Red dye under UV-light irradiation. Impressively, this photocatalyst achieves an 84% degradation of Neutral Red (initial concentration of 20 mg/L) within just five hours. The degradation process relies on active species such as hydroxyl radicals and photo-induced holes, ultimately leading to the mineralization of approximately 70% of Neutral Red into inorganic carbons. ⁽⁹²⁾

The study by D. Liu et al. presents an innovative $\text{TiO}_2\text{-xN}_x/\text{BN}$ composite photocatalyst, which showcases a significant advancement in environmental remediation technologies. This composite is ingeniously engineered by coating nitrogen doped TiO_2 nanoparticles onto the surface of porous BN fibers, creating a material that not only absorbs visible light but also exhibits remarkable efficiency in degrading the dye pollutant Rhodamine B (RhB). Impressively, the composite achieved a degradation efficiency of 97.8% within just 40 minutes of visible light exposure. ⁽⁹³⁾

Chapter 6

Simulation and methodology

6.1 Methodology

Since the exact prices of any of the scaled-up two-dimensional nanomaterials were not available and have not been used in real projects in the industry, a water treatment project was used for the simulation and economic analysis section that employs RO and IX systems for seawater desalination to produce the 5000 m³/d low TDS(total dissolved solids) water for power plants and other uses such as labs and pharmaceutical and medical industries (The schematic diagram is shown in Fig.19). The feeds of this system are provided from Persian Gulf water around Qeshm Island. In this paper, the results of the chemical analysis of Persian Gulf water around Qeshm Island in the Strait of Hormuz are reported. The water samples are taken from various beach places around Qeshm Island in the summer that we use Salakh's data (Table1).

For the economic section of the project, a correction factor of 0.5 was used. This means it was assumed that the RO section, which is the main treatment, was replaced with membranes made from Two-

dimensional nanomaterials, and since their price is much higher than the RO system, 50% was added to the price of the RO system. The economic section of the project was proceeded with this assumption. The WAVE program was used to simulate various parts of this project.

Measured quantity	Tourgan 1	Salakh	Tabl
Ca ²⁺	316	342	342
K ⁺	311	397	173
Mg ²⁺	1341	1305	1015
Na ⁺	8940	9002	7646
Sr ²⁺	6	6	5
Li ⁺	231	252	250
Fe ^{2+*}	0	0	0
Zn ^{2+*}	120	128	130
Mn ^{2+*}	23	28	32
Si ^{4+*}	0	0	0
Cl ⁻	21300	22720	21300
S ²⁻	575	1020	895
SO ₄ ²⁻	1725	3060	2685
F ⁻	0	0	0
pH	8.34	8.01	8.10
TDS (105 °C)	55204	57544	50948
TDS (180 °C)	51300	53500	47400
TDS (550 °C)	45300	47200	41800
Density (g/mL)	1.028	1.028	1.026

All of concentrations are in ppm (mg/L) except those are marked by * which are in µg/L.

Table.1 Analysis of Ion Concentrations and Properties in Tourgan 1, Salakh, and Tabl Water Samples

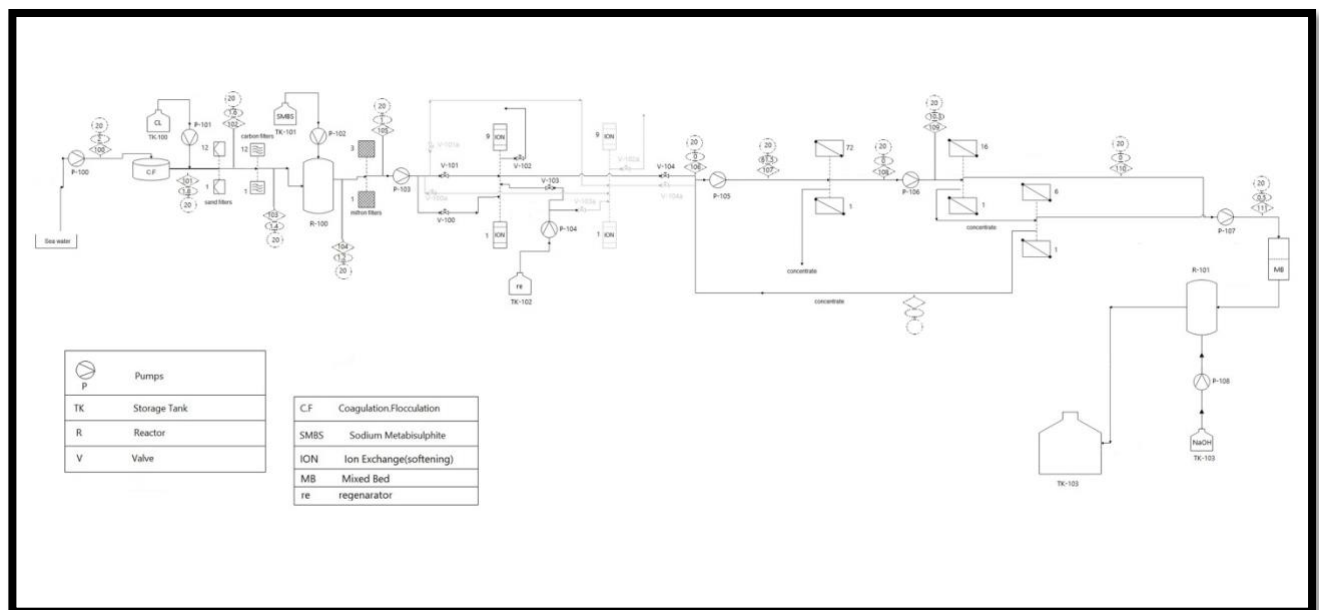


Fig.19 Process Flow Diagram (PFD) of the Plant

6.2 Overall Plant Description

6.2.1 Coagulation-Flocculation

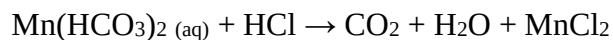
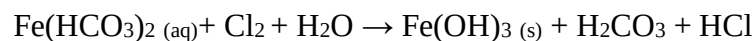
In natural sources like well water, river water, and seawater, suspended solids are present, which can be mineral, organic, or biological. These particles vary widely in size, ranging from less than 1 micron to several centimeters. Coagulation and flocculation are sequential processes used to overcome the forces stabilizing these suspended particles. Coagulation neutralizes particle charges, while flocculation enables them to bind together, making them larger and easier to separate from the liquid. For seawater feed, coagulation and flocculation are necessary to reduce total suspended solids (TSS) and turbidity. In this process, coagulant materials like poly aluminum chloride (PAC) and flocculant materials like polyacrylamide (PAM) are added to the water in a coagulant tank, followed by sedimentation to separate settled material. ⁽⁹⁴⁾

6.2.2 Chlorine Injection

Chlorine is injected into water for two purposes:

1: To remove manganese (Mn^{2+}) and iron (Fe^{2+})

Iron can cause orange, red, or brown fouling (depending on its amount). And also, the presence of manganese in water usually shows itself as black particles. And it may block the membranes and pipelines. Iron dissolved in water is divalent iron Fe^{2+} . After oxidation, dissolved iron becomes trivalent iron Fe^{3+} . In the next step, trivalent iron becomes $\text{Fe}(\text{OH})_3$ iron oxide, which is insoluble and can be easily separated from water by physical filtration. In this process, by injecting a chemical substance into the water, the iron and manganese dissolved in the water are oxidized and become solid particles, and then in the next step, they are separated from the water by physical filtration.



2: Chlorine (Cl_2) has been used for many years to treat water to control microorganisms because of its capacity to inactivate most pathogenic microorganisms quickly. ⁽⁹⁵⁾

6.2.3 Sand Filters

Sand filters are a traditional and widely used method for water treatment, designed to remove suspended particles larger than 100 microns. They are favored for their low cost, effectiveness, and durability, making them popular in industrial applications. ⁽⁹⁶⁾

6.2.4 Carbon Filters

Carbon filtering is a purification method employing activated carbon to eliminate impurities, reduce turbidity, color, and odor through adsorption. It is frequently employed in water treatment processes. Additionally, it aids in removing residual chlorine from preceding steps to prevent damage to membrane polymers in the subsequent RO stage, as chlorine is corrosive. ⁽⁹⁷⁾

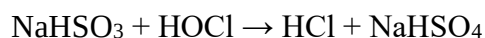
6.2.5 SMBS Injection

In the reverse osmosis process, the RO feed must be dechlorinated to prevent oxidation of the membranes. Sodium Metabisulfite (SMBS) is most common for the removal of free chlorine and as a biostatic. Other chemicals reducing agents exist, e.g. sulfur dioxide, but have not yet been proven cost competitive with SMBS. ⁽⁹⁸⁾

When dissolved in water, sodium bisulfite (SBS) is formed from SMBS:



SBS is then reducing hypochlorous acid according to:



6.2.6 Micron Filters

Micron filters effectively remove dirt, debris, and microscopic particles from water. The pore size of a filter cartridge determines its effectiveness, with smaller micron ratings indicating finer particulate removal. In this case, 5-micron filters have been utilized, offering a specific level of filtration efficiency. ⁽⁹⁹⁾

6.2.7 Softening

Hard water is water that has high dissolved mineral content. Hard water has high concentrations of calcium (Ca^{2+}) and magnesium (Mg^{2+}) ions. Hard water is generally not harmful to one's health but can pose serious plumbing problems in both residential and commercial applications and cause the breakdown in equipment with forming sediments such as CaCO_3 .

The following equilibrium reaction describes the dissolving/formation of calcium carbonate scales:



Calcium and magnesium ions can be easily removed by the ion exchange process.

Eliminating or reducing water hardness is done with a piece of equipment known as a water softener. It is inside this softener where the ion exchange process occurs. A softener is comprised of different components, each having its own unique purpose. The heart of the softener is the mineral tank which is a pressure vessel usually constructed out of fiberglass. These tanks are filled with negatively charged ion exchange resin. The brains of the softener lie in the control valve or softener head as it is commonly referred to. This step has a standby part so that if the online softeners need regeneration, they will enter the regeneration phase and the standby part will start working. ⁽¹⁰⁰⁾

6.2.8 Reverse Osmosis (RO)

In this section, membranes made from two-dimensional nanomaterials are used that operating with a reverse osmosis system.

The membranes used in reverse osmosis systems are typically made of polymers such as polyamide or polysytrene. These membranes are used for filtration and separation of various substances. But in this project, it's assumed that these membranes are made from two-dimensional nanomaterials. This assumption would enhance the efficiency of the membranes and make them more effective in removing contaminants.

The reverse osmosis (RO) process, as its name implies, operates in opposition to natural osmosis and has emerged as a leading method for water purification, particularly in desalination applications. By applying pressure greater than the osmotic pressure to the concentrated solution, typically seawater, the movement of solvent molecules (pure water) is reversed, effectively separating water from impurities. RO systems can be configured as single-pass or two-pass setups. For this project, which requires zero total dissolved solids (TDS) water, a two-stage RO system is employed to meet the desired outcome. ⁽¹⁰¹⁾

6.2.9 Mixed Bed

Mixed bed resin, comprising both cationic and anionic resins, is a crucial component in the water treatment industry. This combined ion exchange resin is utilized to purify water by removing ions until it achieves a high-quality, deionized state. Serving as the final stage of treatment, mixed bed resin ensures thorough purification, resulting in water devoid of any ions. ⁽¹⁰²⁾

6.2.10 NaOH Injection

Sodium Hydroxide (NaOH), commonly known as caustic, stands as the predominant alkaline neutralizing agent in industrial applications today. Praised for its ease of handling, cost-effectiveness, and high efficacy in neutralizing both strong and weak acids, sodium hydroxide plays a vital role in the final step of water treatment. Here, NaOH is injected to balance the pH level, ensuring that the treated water attains a neutral state—neither acidic nor alkaline. This zero TDS water, with a pH of 7 and devoid of ions, finds application across various sectors including power plants, pharmaceuticals, medical, and food industries. ⁽¹⁰³⁾

6.3 Hand calculation

6.3.1 Pumps

For all pumps, these two equations have been used:

For power:

$$Power = \frac{Q * \Delta P}{\text{efficiency}} \quad (1)$$

For suction pressure:

$$P = D * h * g \quad (2)$$

D= density(kg/m³), h=height(m), g=gravitational acceleration=9.8 (m/s²)

p-100

Raw Water Pump:

P_{suction} = 0 bar

Q = 36187 m³/d = 0.42 m³/s

Efficiency = 90%

According to equation (1) → Power = 93 kW

p-101

CL Injection pump: The chlorine tank is located at a height of two meters from the pump so h = 2 m

D_{cl} = 1600 kg/m³

So according to the equation (2)→ $P_{\text{suction}} = 0.3 \text{ bar}$

Efficiency=90%

The amount of chlorine injection is 3 ppm.

So according to equation (1)→ Power =0.03 W

p-102

SMBS Injection pump: The SMBS tank is located at a height of two meters from the pump so $h=2 \text{ m}$

$D_{\text{SMBS}} = 1200 \text{ kg/m}^3$

So according to the equation (2)→ $P_{\text{suction}} = 0.3 \text{ bar}$

Efficiency=90%

The amount of SMBS injection is 3 ppm.

So according to equation (1)→ Power =0.03 W

p-103

In each previous step, a 0.2 bar pressure drop will occur so the suction pressure = $2 - (5 \times 0.2) = 1 \text{ bar}$

ΔP according to the report of WAVE = 0.26 bar

$P_{\text{total}} = 1.26 \text{ bar}$

Efficiency=90%

$Q = 13674 \text{ m}^3/\text{d}$

From equation (1)→ Power =4.6 kW

p-104

Softener regeneration pump: HCL and NaOH in this step will inject.

According to the report of WAVE:

$m_{\text{HCL}} = 1355.15 \text{ kg/d}$ & $D_{\text{HCL}} = 1.49 \text{ kg/m}^3$

$m_{\text{NaOH}} = 1037.9 \text{ kg/d}$ & $D_{\text{NaOH}} = 2130 \text{ kg/m}^3$

Regeneration Injection pump: The regeneration tank is located at a height of two meters from the pump so $h=2 \text{ m}$

So according to equation (2) → $P_{\text{suction}} = 0.42 \text{ bar}$

according to the report of WAVE $\Delta P = 0.26$ bar

$$P_{\text{total}} = 0.68 \text{ bar}$$

$$\text{Efficiency} = 90\%$$

$$\text{From equation (1)} \rightarrow \text{Power} = 0.3 \text{ W}$$

p-105

The pump of Net Feed to Pass 1

From the data in the WAVE $P_{\text{Net Feed to Pass 1}} = 61.5$ bar

$$\text{Efficiency} = 90\%$$

$$Q = 14409 \text{ m}^3/\text{d}$$

$$\text{From equation (1)} \rightarrow \text{Power} = 1081.5 \text{ kW}$$

p-106

The pump of Net Feed to Pass 2

From the data in the WAVE $P_{\text{Net Feed to Pass 2}} = 10.3$ bar

$$\text{Efficiency} = 90\%$$

$$Q = 5777 \text{ m}^3/\text{d}$$

$$\text{From equation (1)} \rightarrow \text{Power} = 76.5 \text{ kW}$$

p-107

Mixed Bed Pump

From the data $Q = 5000 \text{ m}^3/\text{d}$

From the data $P = 0.5$ bar

$$\text{Efficiency} = 90\%$$

$$\text{From equation (1)} \rightarrow \text{Power} = 3.22 \text{ kW}$$

p-108

NaOH Injection pump: The NaOH tank is located at a height of two meters from the pump so $h=2$ m

So according to the equation (2) $\rightarrow P_{\text{suction}} = 0.3$ bar

Efficiency=90%

From equation (1) $\rightarrow \text{Power} = 0.0003$ W

6.3.2 Filters

D =diameter(m), U = linear velocity(m/s) , Q =flow rate(m^3/h) , A =area(m^2) , N =number of filters, h =height(m)

Sand filters

$$D=3.6 \text{ m}$$

$$h=1 \text{ m}$$

$$A_{\text{one filter}} = (\pi/4) \cdot D^2 \cdot h = 10.2 \text{ m}^2$$

$$U=12 \text{ m/s}$$

$$Q=1507.7 \text{ m}^3/\text{h}$$

$$Q=U \cdot A \rightarrow A_T = Q/U \rightarrow A_T = 125.6 \text{ m}^2$$

$$N_{S,F} = A_T / A_{\text{one filter}} \rightarrow N_{S,F} = 12$$

Carbon filters

Are the same as Sand filters so the number of carbon filters are 12

Micron filters

$$Q=1507.7 \text{ m}^3/\text{h}$$

For each $1\text{m}^3/\text{h}$ we should use 10 inches for height and the height of each filter is 40 inches

$$\text{so } N_{F,M} = 1507.7 / 4 \rightarrow N_{F,M} = 377$$

Each 125-micron filter can place in each housing so:

$$N_{\text{housing}} = 377/125 \rightarrow N_{\text{housing}} = 3$$

6.3.3 Softener

The required volume of resin is obtained from the following equation:

$$V_{\text{Resin}} = \frac{QLT}{C} \quad (3)$$

Q=flow rate(m³/h), L=amount of ion removal(eq/L), T=run time(h), C=capacity of resin(eq/L)

In this project, (Amberlite HPR 8400 h) resin has been used so from its sheet:

$$C=4.7 \text{ eq/L (Table2)}$$

From WAVE:

$$L=0.123 \text{ eq/L}$$

$$Q=13675 \text{ m}^3/\text{h}$$

And T= 3 (h) considered

So according to equation (3) $\rightarrow V_{\text{Resin}}=44.7 \text{ m}^3$

$$\text{Also } V_{\text{Softener}} = (\Pi/4) \cdot D^2 \cdot h$$

$$h=1 \text{ m}$$

$$D=2.5 \text{ m}$$

$$\text{So } V_{\text{Softener}}=5 \text{ m}^3$$

The number of softeners ($N_{\text{Softener}} = V_{\text{Resin}} / V_{\text{Softener}} \rightarrow N_{\text{Softener}}=9$)

These are the online softener

There are 9 stand by softeners too

Table.2 Chemical Properties of Amberlite HPR 8400 h

Chemical Properties	
Ionic Form as Shipped	H ⁺
Total Exchange Capacity	≥ 4.7 eq/L (H ⁺ form)
Water Retention Capacity	40.0 – 50.0% (H ⁺ form)

6.3.4 RO (main treatment)

Pass1:

$$N_e = \frac{Q_p}{f \cdot S_E} \quad (4)$$

N_e = number of membranes

Q_p = flow rate(L/h)

f = flux (Lmh)

S_E = active membrane area

from WAVE: $Q_p=248000.8$ L/h

from the following data sheet for membranes (Table 3)

$f= 12-17$ Lmh

according to the membranes model (SW30HRLE-440i)

$S_E=40.9$ m²

So from equation (4) $\rightarrow N_e=505.3$ for $f=12$ Lmh, and $N_e=356.7$ for $f=17$ Lmh

The average of N_e is considered for the number of membranes so

$N_e=431$ (for pass 1)

6 membranes are placed in each pressure vessel so the number of pressure vessels $N_{p,v}=72$

Pass 2:

As the same as pass 1 from equation (4) the number of membranes will be calculated

$Q_p=214775$ L/h

from the following data sheet for membranes (Table 3)

$f= 36-43$ Lmh

according to the membranes model (BW30HRLE-440i)

$S_E=40.9$ m²

So from equation (4) $\rightarrow N_e=146$ for $f=36$ Lmh, and $N_e=122$ for $f=43$ Lmh

The average of N_e is considered for the number of membranes so

$N_e=134$ (for pass 1)

6 membranes are placed in each pressure vessel so the number of pressure vessels $N_{p,v}=22$

In this pass, there are 2 stages in order to increase the efficiency.

The pressure vessels are placed in two stages with the 1:3 ratio

So $N_{p,v-Stage1}=16.5 \approx 16$, and $N_{p,v-Stage2}=5.5 \approx 6$

Table.3 Guidelines for utilizing 8-inch FilmTec™ Elements in water treatment.

Feed Source	RO Permeate	Well Water	Surface Water				Wastewater (Filtered Municipal Effluent or Industrial Effluent)				Seawater			
			With DuPont UF + B-free	Ultrafiltration	Generic membrane filtration or advanced conventional pretreatment	Generic conventional pretreatment	With DuPont UF + B-free	Ultrafiltration	Generic membrane filtration (MBR/MF/UF)	Conventional pretreatment	With DuPont UF + B-free	Well or Open Intake with Ultrafiltration	Open Intake with generic membrane filtration or advanced conventional pretreatment	Open Intake with generic conventional pretreatment
Feed Silt Density Index (%/min)	SDI < 1	SDI < 3	SDI < 2.5	SDI < 2.5	SDI < 3	SDI < 5	SDI < 2.5	SDI < 2.5	SDI < 3	SDI < 5	SDI < 2.5	SDI < 2.5	SDI < 3	SDI < 5
Maximum Element Recovery (%)	30	19	20	19	17	15	15	14	13	12	16	15	14	13
Active Membrane Area	Maximum Permeate Flow, gpd													
365-ft ² elements	10,200	8,500	8,900	8,500	7,200	6,600	6,600	6,300	5,900	5,200	— Not Recommended —			
370-ft ² elements	10,200	8,500	8,900	8,500	7,200	6,600	6,600	6,300	5,900	5,200	8,100	7,800	7,400	7,000
380-ft ² elements	10,700	8,900	9,300	8,900	7,500	6,900	6,800	6,500	6,000	5,300	8,200	7,900	7,600	7,200
390-ft ² elements	10,920	9,200	— Not Recommended —				— Not Recommended —				— Not Recommended —			
400-ft ² elements	11,200	9,300	9,700	9,300	7,900	7,300	7,100	6,800	6,400	5,700	8,800	8,400	8,000	7,600
440-ft ² elements	12,300	10,300	10,700	10,300	8,700	8,000	8,000	7,600	7,100	6,300	9,600	9,200	8,800	8,360
Design Flux Range, gfd (lmh)	21 – 25 (36 – 43)	16 – 20 (27 – 34)	17 – 21 (29 – 36)	16 – 20 (27 – 34)	13 – 17 (22 – 29)	12 – 16 (20 – 27)	12 – 16 (20 – 27)	11 – 15 (19 – 26)	10 – 14 (17 – 24)	8 – 12 (14 – 20)	10 – 12 (17 – 21)	9 – 11 (15 – 19)	8 – 10 (14 – 17)	7 – 10 (12 – 17)
Max. Element Flux, gfd (lmh)	28 (48)	22.7 (39)	24 (41)	22.7 (39)	20 (34)	18 (31)	18 (31)	17 (29)	16 (27)	14 (24)	22 (38)	21 (36)	20 (34)	19 (32)

6.3.5 Reactors

The volume of reactors is calculated with the following equation:

$$V = Q * T \quad (5)$$

$$V = \text{volume (m}^3\text{)}$$

$$Q = \text{flow rate (m}^3\text{/min)}$$

$$T = \text{residence time (min)}$$

So for R-100:

$$Q = 25 \text{ m}^3\text{/min}$$

$$T = 1 \text{ min}$$

$$\text{from equation (5)} \rightarrow V = 25 \text{ m}^3$$

A normal reactor with height=4m and diameter=2m has a volume=12.5 m³

$$\text{So the number of reactors in this step } N_{R-100} = \frac{25}{12.5} \rightarrow N_{R-100} = 2$$

So for R-101:

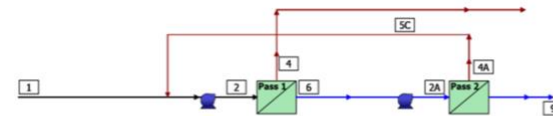
$$Q = 3.4 \text{ m}^3\text{/min}$$

$$T = 1 \text{ min}$$

$$\text{from equation 5} \rightarrow V = 3.4 \text{ m}^3$$

6.4 Simulation

RO Summary Report
RO System Flow Diagram



#	Description	Flow (m ³ /d)	TDS (mg/L)	Pressure (bar)	#	Description	Flow (m ³ /d)	TDS (mg/L)	Pressure (bar)
1	Raw Feed to RO System	13,674	42,144	0.0	2A	Net Feed to Pass 2	5,777	154.4	10.3
2	Net Feed to Pass 1	14,409	40,050	61.5	4A	Total Concentrate from Pass 2	774.9	1,119	6.0
4	Total Concentrate from Pass 1	8,646	66,648	60.1	5C	Concentrate Recycle from Pass 2 to Pass 1	774.6	1,120	6.0
6	Total Permeate from Pass 1	5,780	154.3	0.0					
9	Net Product from RO System	5,005	4.85	0.0					

RO System Overview

Total # of Trains	1	Online =	1	Standby =	0	RO Recovery	36.6 %
System Flow Rate	(m ³ /d)	Net Feed =	13,674	Net Product =	5,005		

Fig.20 RO System Flow

Table.4 RO Flow Table for Pass 1

Stage	Element	Element Name	Recovery (%)	Feed Flow (m ³ /d)	Feed Press (bar)	Feed TDS (mg/L)	Conc Flow (m ³ /d)	Perm Flow (m ³ /d)	Perm Flux (LMH)	Perm TDS (mg/L)
1	1	SW30HRLE-440i	10.6	200.1	61.2	40,050	179.0	21.2	21.6	80.15
1	2	SW30HRLE-440i	9.9	179.0	61.0	44,777	161.2	17.8	18.1	104.8
1	3	SW30HRLE-440i	9.0	161.2	60.7	49,688	146.8	14.5	14.7	139.5
1	4	SW30HRLE-440i	7.8	146.8	60.6	54,552	135.5	11.4	11.6	188.9
1	5	SW30HRLE-440i	6.5	135.5	60.4	59,119	126.7	8.78	9.0	259.0
1	6	SW30HRLE-440i	5.2	126.7	60.2	63,189	120.1	6.63	6.8	358.0

Table.5 RO Flow Table for Pass 2

Stage	Element	Element Name	Recovery (%)	Feed Flow (m ³ /d)	Feed Press (bar)	Feed TDS (mg/L)	Conc Flow (m ³ /d)	Perm Flow (m ³ /d)	Perm Flux (LMH)	Perm TDS (mg/L)
1	1	BW30HRLE-440i	12.5	361.1	10.0	154.4	316.2	45.0	45.8	2.80
1	2	BW30HRLE-440i	13.5	316.2	9.4	175.9	273.5	42.7	43.5	3.22
1	3	BW30HRLE-440i	15.0	273.5	9.0	202.8	232.5	41.0	41.7	3.69
1	4	BW30HRLE-440i	17.1	232.5	8.6	237.9	192.9	39.7	40.4	4.24
1	5	BW30HRLE-440i	20.1	192.9	8.3	285.9	154.2	38.7	39.5	4.89
1	6	BW30HRLE-440i	24.7	154.2	8.1	356.5	116.1	38.1	38.8	5.74
2	1	BW30HRLE-440i	11.2	309.5	7.7	471.7	274.9	34.6	35.3	5.77
2	2	BW30HRLE-440i	11.8	274.9	7.3	530.3	242.5	32.5	33.1	6.45
2	3	BW30HRLE-440i	12.6	242.5	6.9	600.4	211.9	30.6	31.2	7.22
2	4	BW30HRLE-440i	13.7	211.9	6.6	685.9	182.9	29.0	29.5	8.11
2	5	BW30HRLE-440i	15.1	182.9	6.4	793.2	155.4	27.6	28.1	9.23
2	6	BW30HRLE-440i	16.9	155.4	6.1	932.2	129.2	26.3	26.8	10.73

Chapter 7

Economic Analysis

To determine the expenses associated with pumps, reactors, and filters, I referenced the diagrams from Ulrich's book "A Guide to Chemical Engineering Process Design and Economics." These diagrams provide insights into equipment materials and operating pressures. However, since the costs in the book were based on 1982 figures, I adjusted them to reflect 2024 values using a conversion factor derived from the chemical engineering index, which stood at 803.4/315.

a CE index(2023)/ CE index(1982) = 803.4/315								
(US \$)=500000 Rial								
EQUIPMENTS		number	capacity	purchase price, 1982 (US \$)	a	purchase price, 2023 (US \$)	bare module factor, F _{BM}	CBM, stainless steel (US \$)
								(US \$)
pumps								
	p_100, centrifugal	1	93 Kw	18500	2.6	47175	4.2	198135
	p_101, centrifugal	1	0/03 W	negligible	2.6	negligible	4.2	negligible
	p_102, centrifugal	1	0/03 W	negligible	2.6	negligible	4.2	negligible
	p_103, centrifugal	1	4/6 Kw	5500	2.6	14025	4.2	58905
	p_104, centrifugal	1	0/3 W	1200	2.6	3060	4.2	12852
	p_105, centrifugal	1	1081/47 Kw	100000	2.6	255000	4.2	1071000
	p_106, centrifugal	1	76/5 Kw	15000	2.6	38250	4.2	160650
	p_107, centrifugal	1	3/22 Kw	5000	2.6	12750	4.2	53550
	p_108, centrifugal	1	/0003 W	negligible	2.6	negligible	4.2	negligible
	suction pressure of all pumps < 1 barg							
	sub total			145200				1555092
Reactors								
	R-100	2	D=2(m)	70000	2.6	182000	2.9	1055600
	R-101	2	D=1(m)	35000	2.6	91000	2.9	527800
	sub total							1583400
Filters								
	sand filters	12	A=10(m2)	3100	2.6	96720	2.8	270816
	carbon filters	12	A=10(m2)	3100	2.6	96720	2.8	270816
	micron filters	377	A=0/02(m2)	1	2.6	980.2	2.8	2744.56
	sub total							544376.6
IX								
	Softening	18				280		5040
	Mixed bed	1				280		280
	Resin Amberlite	45	m3					
		1592.16	ft3	1987	\$/ft3			3163621.92
	sub total							3168941.92
RO								
	Pass 1	432				800		345600
	Pass 2	132				400		52800
	sub total (RO)							398400
	sub total (RO 2D-Nano)							597600
Tanks								
	TK-103	1	V=5000(m3)	550000	2.6	1430000	1.9	2717000
total bare module cost								
contingency and fee (18 % of total actual bare module)								
total "process module" or "battery-limits" cost								
auxiliary and offsite facilities (30% of total bare module cost)								
total "grass-root" plant capital cost								
							IF	14332665.76
							Iw	2149899.865
							IL	0
							IT	16482565.63

Fig.21 I_F Calculation Excel sheet

7.1 Fixed Capital Cost (I_F)

Fixed capital cost (I_F) estimate requires updated prices (the effect of inflation) for all the equipment, properly sized, and installed. The objective is to get within +/- 30% of actual costs. (Fig.21)

Based on figure 15, the computational results obtained in Excel are as follows:

Cost of Pumps = \$1,555,092

Cost of Reactors = \$1,583,400

Cost of Filters = \$544,376.6

Cost of IX = \$3,168,941.9

Cost of RO(2D-Nano) = \$597,600

Cost of Tanks = \$2,717,000

Total bare module cost = Cost of Pumps + Cost of Reactors + Cost of Filters + Cost of IX +
Cost of RO(2D-Nano) + Cost of Tanks So $\Sigma_{\text{costs}} = \$7,449,410.5$

Contingency and fee (18 % of total actual bare module) = \$1,340,893.9

Auxiliary and offsite facilities (30% of total bare module cost) = \$2,234,823

Total "grass-root" plant capital cost (Total bare module cost + Contingency and fee +
Auxiliary and offsite facilities) so $\Sigma_T = \$11,025,127.5$

I_F = Total "grass-root" plant capital cost + 30% so,

$$I_F = \$14,332,665.7$$

7.2 Total Investment (I_T)

$$I_T = I_F + I_W + I_L$$

$$I_F = \$14,332,665.7$$

$$I_W = 15\% \text{ of } I_F \text{ so } I_W = \$2,149,899.8$$

we don't have any I_L so $I_L = 0$ so,

$$I_T = \$16,482,565.6$$

7.3 Annual Total Expenses (A_{TE})

The annual total expenses (ATE) are calculated by adding the annual direct manufacturing cost (ADME), the annual indirect manufacturing expenses (AIME), and the annual general expenses (AGE).

$$A_{TE} = A_{DME} + A_{IME} + A_{GE}$$

A_{DME}

Labor costs

From Ulrich book this plant needs 15 operators for 3 shifts.

The amount of salary that should be paid for every operator is \$3,250 per month.

For one year, cost of operators: (15 operators/month) * (\$3,250 /month) * (330 day/ 1 year) = \$585,000

Utility costs

The total power of pumps = 1257.9 kW

The price of industrial electricity = 2 cent /kWh

Total price \$/Year = \$21,135.6

Maintenance & repair	6%	of fixed capital cost	\$859,960
Operating supplies	15%	of maintenance cost	\$64,497
Laboratory expense	15%	of labor cost	\$87,750
Patents & royalties	3%	of ATE	We don't have

*Assume maintenance cost is 3 % of fixed cost.

A_{IME}

Overhead fringe benefits, unemployment insurance (UI) for employees

60% of the sum of all the labor and maintenance costs = \$608,988

Insurance & property taxes 2% of the fixed capital cost = \$ 286,653.3

Depreciation Costs These are expenses that an accountant includes as a tax incentive. (fixed cost/plant life) = \$14,332,665.7/15 = \$955,511

A_{GE}

Administrative costs 25% of plant overhead = \$152,247

Research & development 5% of ATE (ATE = \$3,469,495 without this item) = \$173,474.7

Distribution & sales 10% of ATE (ATE = \$3,469,495 US without this item) = \$346,949.5

$$A_{TE} = \$4,142,166$$

7.4 Annual Total Sales (A_S)

In this plant, 1650000000 Liter zero TDS water is produced annually so

$$Q=1650000000 \text{ L/Year}$$

The price of this type of water is 0.09 \$/L that is sold to power plants, pharmaceutical and food industries.

So, the annual sales $A_S = (1650000000 \text{ L/Year}) * (0.09 \text{ $/L}) = 148,500,000 \text{ $/Year}$

7.8 Annual Net Cash Income

$$A_{NCI} = A_{CI} - A_{IT}$$

$$A_{CI} = A_S - A_{TE} = \$148,500,000 - \$4,142,166 = \$144,357,834$$

$$A_{IT} = (A_{CI} - A_D - A_I) * t$$

$$A_I = 0$$

$$A_D = I_F / \text{plant life}$$

$$t = 35\%$$

$$A_{IT} = \$50,190,813$$

$$A_{NCI} = \$94,167,021$$

The economic analysis calculations based on the mentioned data have been conducted using Microsoft Excel. the summary of the results are:

1: Payback Period (PBP) =1 year

2: Discounted Cash Flow Rate of Return (DCFRR) =35%

So, 2D-Nanomaterials are profitable for water purification.

	14332665.76		148500000							
yr	I_F	I_W	A_S	A_{TE}	$A_{CF}=A_{OC}-A_{TE}-I_W$	$A_D=I_F/15$	A_I	$A_{IT}=0.35^*(A_{CF}-A_D-A_I)$	$A_{NCF}=A_{CF}-A_{IT}$	$CumA_{NCF}$
1	4777555.253	0	0	0	-4777555.253			0	-4777555.253	-4777555.253
2	4777555.253	0	0	0	-4777555.253			0	-4777555.253	-9555110.507
3	4777555.253	0	0	0	-4777555.253			0	-4777555.253	-14332665.76
4	0	2149899.864	74250000	50190813	21909287.14	955511.0507	0	7333821.63	14575465.51	242799.7461
5	0		148500000	50190813	98309187	955511.0507	0	34073786.58	64235400.42	64478200.16
6	0		148500000	50190813	98309187	955511.0507	0	34073786.58	64235400.42	128713600.6
7	0		148500000	50190813	98309187	955511.0507	0	34073786.58	64235400.42	192949001
8	0		148500000	50190813	98309187	955511.0507	0	34073786.58	64235400.42	257184401.4
9	0		148500000	50190813	98309187	955511.0507	0	34073786.58	64235400.42	321419801.8
10	0		148500000	50190813	98309187	955511.0507	0	34073786.58	64235400.42	385655202.3
11	0		148500000	50190813	98309187	955511.0507	0	34073786.58	64235400.42	449890602.7
12	0		148500000	50190813	98309187	955511.0507	0	34073786.58	64235400.42	514126003.1
13	0		148500000	50190813	98309187	955511.0507	0	34073786.58	64235400.42	578361403.5
14	0		148500000	50190813	98309187	955511.0507	0	34073786.58	64235400.42	642596803.9
15	0		148500000	50190813	98309187	955511.0507	0	34073786.58	64235400.42	706832204.3
16	0		148500000	50190813	98309187	955511.0507	0	34073786.58	64235400.42	771067604.8
17	0		148500000	50190813	98309187	955511.0507	0	34073786.58	64235400.42	835303005.2
18		-2149899.864	148500000	50190813	100459086.9	955511.0507	0	34826251.53	65632835.33	900935840.5

Fig.22 Cumulative Net Cash Income

1								
i=0/1			i=0/3			i=0/35		
$f_d=1/(1/1)^j$	A_{OCI}	$CumA_{OCI}(i=10\%)$	$f_d=1/(1/3)^j$	A_{OCI}	$CumA_{OCI}(i=30\%)$	$f_d=1/(1.35)^j$	A_{OCI}	$CumA_{OCI}(i=35\%)$
0.91	-4343232.048	-4343232.048	0.77	-3675042.503	-3675042.503	0.74	-3538929.817	-3538929.817
0.83	-3948392.771	-8291624.82	0.59	-2826955.771	-6501998.274	0.55	-2621429.494	-6160359.312
0.75	-3589447.974	-11881072.79	0.46	-2174581.362	-8676579.636	0.41	-1941799.625	-8102158.937
0.68	9955239.059	-1925833.735	0.35	5103275.623	-3573304.013	0.30	4388209.568	-3713949.369
0.62	39885129.81	37959296.08	0.27	17300460.93	13727156.92	0.22	14325361.6	10611412.23
0.56	36259208.92	74218505	0.21	13308046.87	27035203.79	0.17	10611378.96	21222791.19
0.51	32962917.2	107181422.2	0.16	10236959.13	37272162.93	0.12	7860280.713	29083071.91
0.47	29966288.37	137147710.6	0.12	7874583.948	45146746.88	0.09	5822430.158	34905502.06
0.42	27242080.33	164389790.9	0.09	6057372.268	51204119.14	0.07	4312911.228	39218413.29
0.39	24765527.57	189155318.5	0.07	4659517.129	55863636.27	0.05	3194749.058	42413162.35
0.35	22514115.98	211669434.5	0.06	3584243.946	59447880.22	0.04	2366480.784	44779643.13
0.32	20467378.16	232136812.6	0.04	2757110.727	62204990.95	0.03	1752948.729	46532591.86
0.29	18606707.42	250743520	0.03	2120854.406	64325845.35	0.02	1298480.54	47831072.4
0.26	16915188.56	267658708.6	0.03	1631426.466	65957271.82	0.01	961837.4368	48792909.84
0.24	15377444.15	283036152.7	0.02	1254943.435	67212215.25	0.01	712472.1754	49505382.01
0.22	13979494.68	297015647.4	0.02	965341.1041	68177556.36	0.01	527757.167	50033139.18
0.20	12708631.53	309724279	0.01	742570.0801	68920126.44	0.01	390931.2348	50424070.42
0.18	11804642.34	321528921.3	0.01	583634.3232	69503760.76	0.00	295878.4488	50719948.87

Fig.23 Discounted Cash Flow

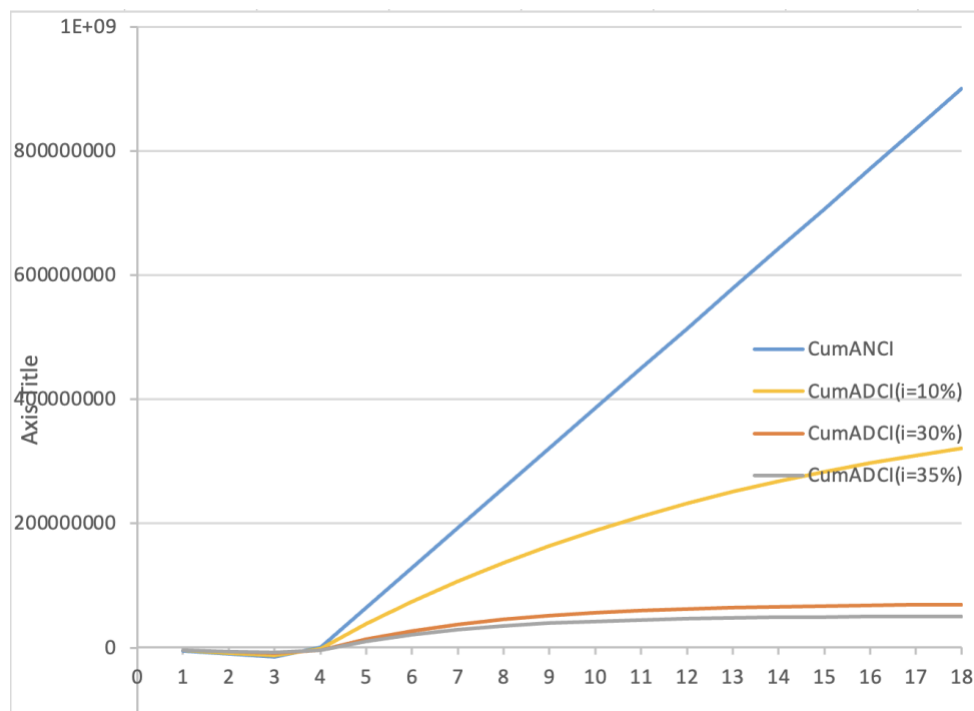


Fig.24 Cumulative Annual Cash Flow Chart

Chapter 8

Challenges & Recommendation for future works

8.1 Challenges

Since two-dimensional nanomaterials are new materials in water purification and are still in the research phase, they face a series of challenges and constraints in water treatment, including:

- **Manufacturing Costs:** The production of many 2D nanomaterials is still relatively expensive compared to traditional materials, necessitating cost reductions for large-scale industrial applications.
- **Sustainability:** The long-term viability of 2D nanomaterials, both in terms of production and application, must be considered to prevent substance recontamination.
- **Biocompatibility:** Since water treatment is essentially a decontamination process, the biocompatibility of 2D nanomaterials must be evaluated to ensure they do not introduce new contaminants into the environment.

Technological and Operational Stability: Improving methods to maintain specific nanochannels with long-term operational stability is crucial for effective water transport and high-performance solar desalination. ⁽¹⁰⁴⁾

8.2 Recommendation for Future Works

8.2.1 Multifunctional Nanomaterials: Develop multifunctional 2D nanomaterials that can simultaneously perform adsorption, catalysis, and antimicrobial activities. Integration of different functionalities into a single nanomaterial can enhance overall water treatment efficiency and reduce the complexity of treatment systems.

8.2.2 Scale-up and Commercialization: Scale up the synthesis and production of 2D nanomaterials for large-scale water treatment applications. Develop scalable fabrication techniques and manufacturing processes to facilitate the commercialization and widespread adoption of nanomaterial-based water treatment technologies.

8.2.3 Integration with IoT and AI: Integrate 2D nanomaterial-based water treatment systems with artificial intelligence (AI) algorithms for real-time monitoring and control. Develop smart water treatment platforms capable of autonomous operation, adaptive optimization, and predictive maintenance.

8.2.4 Resource Recovery: Explore the potential for resource recovery from wastewater using 2D nanomaterials. Develop nanomaterial-based technologies for the recovery of valuable resources such as metals, nutrients, and energy from wastewater streams, contributing to the circular economy and sustainable resource management.

Conclusion

In this thesis, we have explored the significant potential of two-dimensional nanomaterials in addressing the critical challenges of water and wastewater treatment. The unique physical and chemical properties of materials such as graphene, metal-organic frameworks, and molybdenum disulfide, including their high surface area and reactivity, make them exceptionally effective in removing contaminants from water. While there are other materials in this field that are cheaper than two-dimensional nanomaterials, the enhanced performance and effectiveness of nanomaterials often justify their higher cost. Furthermore, the long lifespan and recoverability of some nanomaterials can offset their initial expenses in the long term. Additionally, many other materials like membrane

filtration, which were initially not cost-effective, have found more economical ways for water treatment with technological advancements. This indicates that with technological progress, two-dimensional nanomaterials can also achieve more cost-effective methods for water purification and scaling them up. The design and economic analysis of a water purification plant for the Persian Gulf region further underscores the practical and commercial viability of these nanomaterials. As we continue to face global water scarcity and pollution, the continued development and scaling of these nanotechnologies will be critical. The insights gained from this study encourage further exploration and optimization of 2D nanomaterials to meet the world's growing water needs responsibly and innovatively.

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