Design and Modelling of Water Filtration Assembly Incorporating Graphene Embedded Membrane

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Abstract

The current study is based on design of the latest innovation in water treatment technology. In this study inclusion of graphene oxide particles in the Polyether Sulfone (PES) hollow fiber membrane is studied and a filtration assembly is designed along with engineering drawings for it, taking into consideration of local conditions. Optimum methodologies were selected after the conduction of cost-benefit analysis and detailed literature review. Flash Graphene technique is recommended over Improved Hummer's technique due to its fast results and scalability. PES hollow fiber membranes are suitable and have a relatively good performance for water treatment. Our review showed major performance improvements in the PES membranes after incorporating 0.5% by weight of graphene oxide. These improvements include, but are not limited to improved flux, hydrophilicity, life, bacteriological and viral reductions and less clogging. Information regarding demand and required output was inputted in the WAVE software by Dupont to model the required membrane characteristics. The surface area was calculated by interpolating data from AMI membranes. The graphene-enhanced membrane assembly was found to provide, in theory, the same amount of water purification performance compared to pure PES membranes all while having a 90% reduced physical size. The assembly was designed on AutoCAD and SolidWorks and includes a sand filter in the first stage, GO-MEM in the second stage, with three valves and operation modes. Backwashing requirement is minimal depending upon feedwater and the optimal lifespan is of two years. This designed filter is a first step towards advance membrane filtration of drinking water with improved performance.

Keywords: *Drinking water treatment; GO-MEM, Polyether Sulfone (PES) hollow fiber membrane, Flash graphene technique, WAVE software*.

1. Introduction

Globally, membrane technology has greatly increased its share in the water treatment technology market over the past few years due to its efficient operation, modular structure, low power consumption, environmentally friendly operation, and minimal chemical requirement. While there are many advantages over traditional water treatment methods and the ability to perform a variety of functions, membrane technology has its disadvantages when it comes to water treatment i.e., fouling, short life, hydrophobicity of used polymers, etc. [1]. Also, depending on the composition of the solution, filtering of small particles (e.g., bacteria and viruses) may not be achieved. Therefore, the development of highly efficient membranes to overcome these challenges and/or improved performance is an active field of research for the past decades and nanotechnology plays a major role in it. Advances in membrane formation, transformation and development of existing membranes can be employed to create membranes with improved efficiency and effectiveness. Triple Water Filters in our homes, schools, and workplaces have less than optimal performance, due to the high maintenance required.

Water scarcity is already affecting all continents, and water use has grown worldwide more than twice the rate of population growth over the past century, with a greater number of countries reaching the limit at which water services can be delivered sustainably, especially in those arid zones. More than two billion people live in countries with high water stress.

The Earth just has 1% usable water, and it is distributed unfairly. Over 700 million people face intense water scarcity [2]. Climate change and pollution are making the problem worse. The demand for water globally is growing fast. Attitudes towards water consumption and management must be changed and newer technologies must be adopted. Based on these factors the current study is trying to address the problem that is:

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"The world is quickly running out of water and the need for recycling existing water using newer and improved technology is rapidly increasing to cater for demand. Existing technology including water desalination, RO membranes, and home-based units have lots of limitations. A big shift into the next generation of technology is needed."
To address this problem the current study is designed to outline a method to prepare a polyethersulfone (PES) membrane incorporating turbostratic graphene-oxide by phase inversion technique. Then to produce the design and 3D model of the water filtration assembly for the incorporation of the membrane using Computer-Aided Engineering Software (CAE) and to model the properties and optimum configurations of the water filtration assembly for treatment efficiency [3].
The study was conducted in two phases. The first phase involved a literature review and selection of the latest and optimal methods to produce the desired membrane. This is to ensure the final product is feasible and practical according to local conditions. This phase involved consultation with experts in School of Chemical and Material Engineering (SCME, NUST). Flash graphene and PES hollow fiber membranes were selected. The second phase involved the design of a water filtration assembly through AutoCAD and SolidWorks, including both the 3D model and engineering drawings [4]. This work is a blueprint for future researchers and engineers to produce it in real life.
Graphene is a new material discovered in 2004 at the University of Manchester by Andre Geim and Konstantin Novoselov. Graphene is now considered a wonder material. It is the strongest, lightest, most thermal, and electrically conductive material out there. A single sheet of graphene covering the entire area of a football pitch would weigh less than 1 gram. It has a tensile strength of 130 GPa (200 times stronger than structural steel). It is also very flexible and is 35% less electrically resistive than copper, and 5 times better at conducting heat compared to it [5].
Every era of human technological development has been marked by a material. Some have even gone as far as to say that the next age will be the Graphene Age [6]. This is illustrated in Fig. 1.

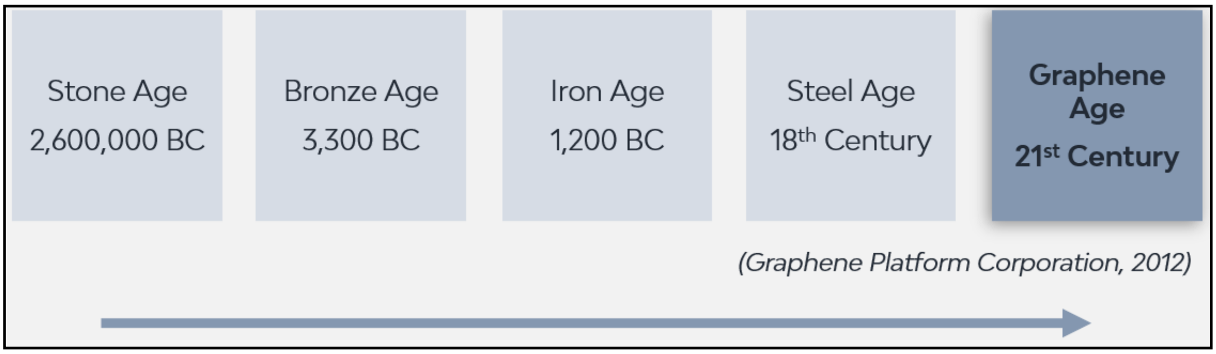


Fig. 1: Eras of Human Technological Development

The discovery of graphene had piqued the interest of many environmental scientists around the globe. The material was tested for its properties regarding suitability for use in water treatment. It was shown from various studies that graphene has a lot of potential in this field, enhancing treatment technologies in many ways. It shows great promise.
One study was done on graphene oxide and its effects on PES membranes. Compared to pure membranes, the graphene incorporated membranes showed enhanced water flux, salt rejection, antimicrobial properties, and even heavy metal adsorption [7]. Another study used Molecular Dynamic Simulations using software to show selective adsorption by graphene oxide, namely, LAMMPS [8].

1.1. Ultrafiltration (UF)

UF is a pressure driven process against a semi-permeable membrane barrier that filters out solids and microorganisms. It produces pure water. Suspended solids are retained at the barrier while water passes through it. UF is not entirely different from RO, MF, or NF, except for the size of membrane pores themselves. Ultrafiltration has a pore size of about 0.002 to 0.1 microns [9].

1.2. Polyether Sulfone Membrane

Recently, a new type of membrane made of polyether sulfone (PES) has become commercially available. Comparisons between PES and polyvinylidene fluoride (PVDF) showed that PES membranes allow a higher rate of filtration and clogged slower [10]. Therefore, the use of PES membranes is recommended and was picked for current study.

1.3. Graphene Oxide (GO) Embedded Membranes

Embedding GO serves as an effective selective barrier and can achieve higher water permeability without compromising the selectivity of membranes [11]. This is why the addition of graphene oxide particles into membrane polymers greatly increases their performance. Extensive lab tests and experiments have shown optimal addition of graphene particles will result in a membrane better in many orders of magnitude.

2. Methodology

Two methods were shortlisted to produce graphene oxide. They include the improved Hummer's method and the Flash graphene method. Hummer's approach is currently being used widely in labs while the flash graphene method has potential for large-scale use, owing to its simplicity and fast results [12]. Considering the benefits of both methods to be constant, the flash graphene method has lower costs compared to improved hummer's method. Thus, it has a higher benefit-cost ratio (BCR).

A cost-benefit analysis was conducted between GO-MEM and TWF. Fig. 2 below illustrates its details. Incremental cash flow analysis showed the benefit-cost ratio to be 0.267 which indicated that GO-MEM is the better option for the local market.

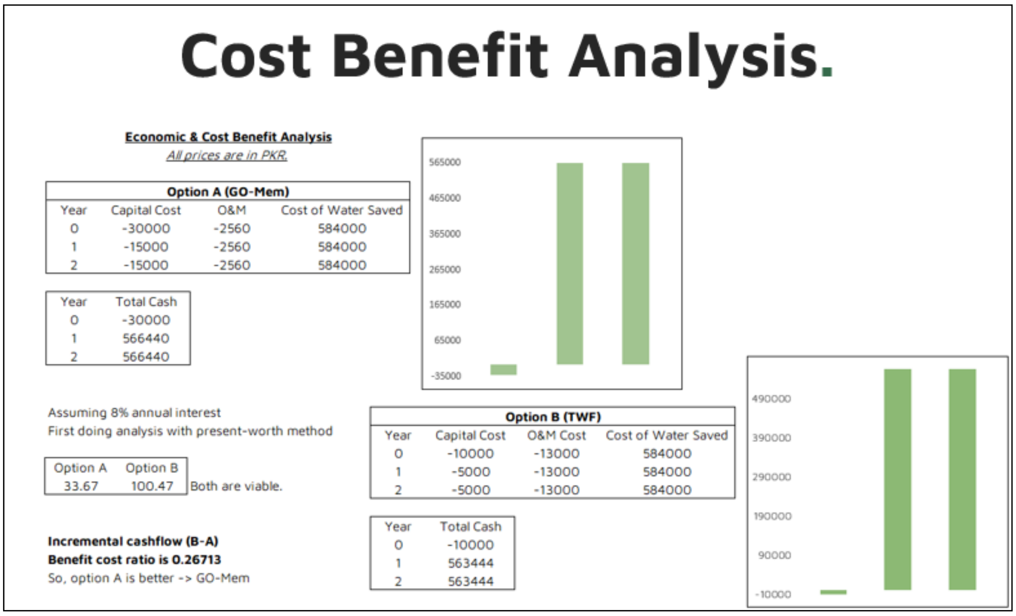


Fig. 2: Cost-Benefit Analysis between GO-MEM and TWF

1.4. Flash Graphene Method

This method is one of the advanced methods of graphene oxide synthesis and it involves a process in which the electric current is passed through a carbon-based material. This process converts the amorphous carbon into graphene by using the energy with the help of the electrical discharge. The material other than carbon present in the source is being transformed into a volatile gas [13]. This method produces high-quality graphene, and the process is so quick that it does not allow the atoms to align due to electrostatic interaction which enables us to extract the individual layers of graphene without any disturbances in its structure.

Gram-scale graphene is produced almost instantly from any carbon source and the process uses no furnace, solvents, or reactive gases. Yield depends on the carbon content of the source; if a high carbon source is used, the yield can range from 80 - 90% with a 99% carbon purity.

Estimated energy for conversion of high carbon materials into flash graphene [14].

$$\mathbf{E = (V_1 - V_2)(V_1 + V_2) \times (C/2M)} \quad (1)$$

Where V_1 and V_2 are voltage before and after flash, E is energy per gram, C is capacitance, M is mass per batch.

The calculated energy is thus,

$$\mathbf{E = 7.2\ kJ/g} \quad (2)$$

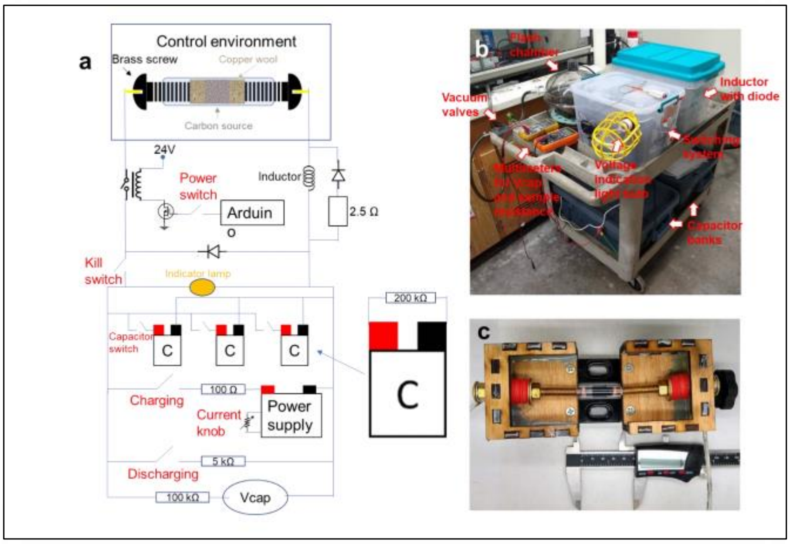


Fig. 3: Circuit

Fig. 3 above shows the electric circuit design can be used for this method in real scenario, and the methodology is outlined below.

1. The method involves placing the carbon-based material inside of a quartz tube by placing two metallic screws on both of its sides that will act as the electrodes.
2. The compression is made by using the copper-wool plugs that will allow the carbon-based material to get in contact with the electrodes.
3. The pressure is applied and controlled via a pressure vice that will also minimize the resistance that is good for flash reactions.
4. The controller and mechanical relay are used to maintain the voltage pulse.
5. This entire reaction is carried out in a low-pressure container i.e., a vacuum desiccator.
6. A set of capacitors would be required to produce a minimum combined capacitance of 0.22 F.
7. A single three-phase generator would be used for producing the AC power for this circuit.

The carbon-based material required for this process can be taken from inexpensive sources such as coal, petroleum coke, biochar, carbon black, discarded food, rubber tires, and mixed plastic waste [15]. The electrical energy required for this method is calculated to be 7.2 kJ/g which makes flash graphene suitable for use in bulk plastic, metals, paints, concrete, and other building materials.

1.5. Targeted Pollutants and lab tests

Five drinking water pollutants were targeted in this study namely E. Coli, turbidity, TDS, arsenic, and lead. The data was required to run the membrane feasibility simulations and models. A few lab tests were carried out to assess NUST drinking water. Turbidity, TDS, temperature, pH, EC, free chlorine, and E. Coli tests were conducted in the lab. Arsenic and lead values were obtained from recent work done at institute.

1.6. Dupont WAVE

For the modeling and simulation of proposed designed assembly, software named WAVE is used. Water Application Value Engine (WAVE) is a fully integrated modeling tool that incorporates three technologies i.e., ultrafiltration, reverse osmosis, and ion exchange. In the graphene oxide embedded membrane, an ultrafiltration technique would be used that helps to utilize this software. This software is a comprehensive tool that simplifies various design processes of proposed assembly and enables to minimize the cost and time that will be required in the designing of a filtration assembly with high accuracy.

1.6.1. Modeling of our Design

Before starting the actual modelling of data, the first thing to do is to set various default setting in the system as per need. The measuring units that have been taken are the standard metric system that remains consistent throughout the calculations and are shown in Fig. 4 and Fig. 5.

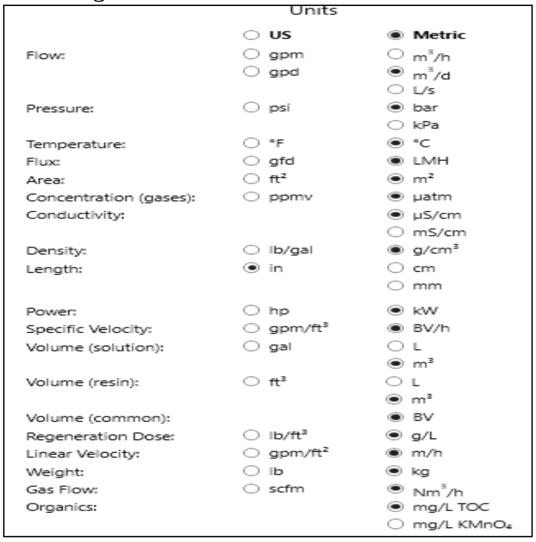


Fig. 4: Setting Units in WAVE

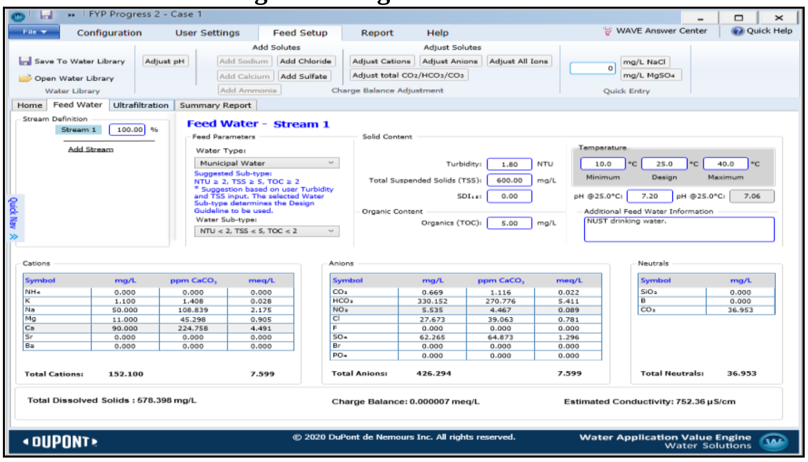


Fig. 5: WAVE Interface

Then, the software requires some of the water characteristic values to be entered so that to get a more accurate result. Different water-type options are available in the software and out of which the municipal water type is used. The average input water flowrate is taken as 14.6 m^3/day which is the normal tap water flowrate, and this value was taken from the literature. This is the average flow that is generated from the faucets that are normally used in our homes and offices. The values required for the turbidity, temperature, total suspended solids, and the total organic content were taken from the lab tests that were practically performed in the laboratory. For experimental purposes, three different water samples were taken from the IESE building from separate taps.
The anion and cation values that we needed for the water input are taken from the reports of the Pakistan Council of Research in Water Resources [16]. Some literature values have also been used such as that of the arsenic and lead values as their tests were not performed practically due to some technical issues.

2. Results and Discussion

After all the values have been entered in WAVE interface, the system will run its calculations and generates a report for filtration system. Two types of reports are generated from it, one is the summary report which provides an overview of different components that are being used in the system [17]. The other one is the detailed PDF report that shows all the calculations and values that have been performed in the design.

UF System Overview

Module Type		IntegraFlux SFD-2860XP			
# Trains		Online =	1	Standby =	0
				Redundant =	0
# Modules		Per Train =	1	Total =	1
System Flow Rate	(m³/d)	Gross Feed =	16.4	Net Product =	14.4
Train Flow Rate	(m³/d)	Gross Feed =	16.4	Net Product =	14.4
UF System Recovery	(%)	88.38			
TMP	(bar)	0.08 @ 10.0 °C		0.06 @ 25.0 °C	
Utility Water		Forward Flush:	Pretreated water	Backwash:	UF filtrate water
		CEB Water Source:	UF filtrate water	CIP Water Source:	UF filtrate water

UF Operating Conditions

	Duration	Interval	Flux/Flow
Filtration:	90.0 min	92.9 min	-
Instantaneous			
1 Online Trains			13 LMH
1 Total Trains			13 LMH
Average			13 LMH
Net			12 LMH
Backwash	2.9 min	92.9 min	100 LMH

Fig. 6: WAVE Results

Furthermore, the membrane area, length, diameter, and weight that would be required for this design has been calculated by using this software. But there is an issue relating to these values as the system's membrane specifications do not incorporate graphene into it and due to which few adjustments are made in these values.

These reports will help to understand the input concentrations of feed water and the output feed water values that would be obtained. Besides the general modeling to check the efficiency and level of filtration that the designed system will conduct, the detailed cost analysis can also be performed by using this software [18].

For the cost analysis, the currency units are converted to PKR and the electricity values are taken in kWh. By the calculations performed, it has been calculated that the average operating cost of the GO-embedded membrane-based system would be 6.2 PKR/day and if the backwash technique has also been used with the system, then the additional cost of 0.43 PKR/day would be added to the daily operational cost.

2.1. Autodesk AutoCAD

Fig. 7 shows the PFD that was made for proposed design. The PFD was converted into an initial 2D design that is shown in Fig. 8. Purification / normal operation is in steps 1-3. Water first enters the assembly into the sand filter from the feed tank. After this primary treatment, it will move to the GO-MEM through a perforated layer [19]. The membrane will work on home water tap pressure (0.2 bars) and produce clean water at the end. For backwashing, the same line will be used, clean water will enter the GO-MEM from the opposite side and leave the assembly through steps 4-6.

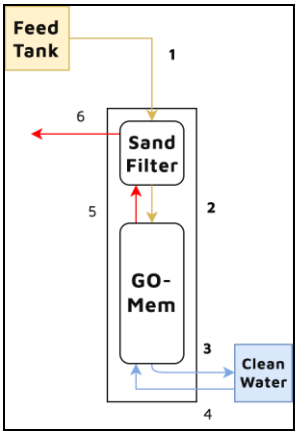


Fig. 7: Process Flow Diagram (PFD)

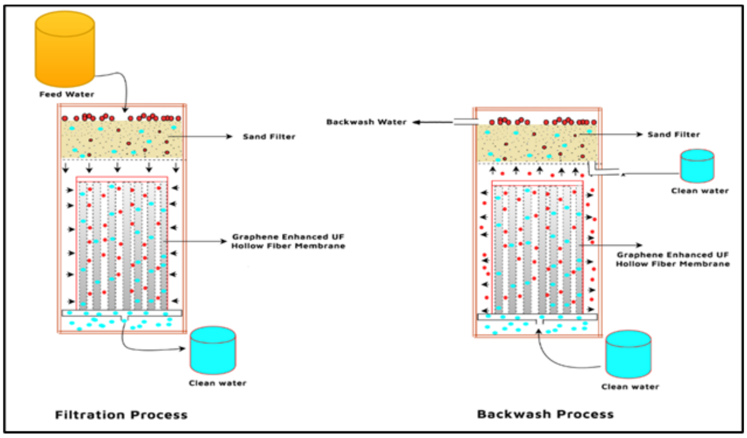


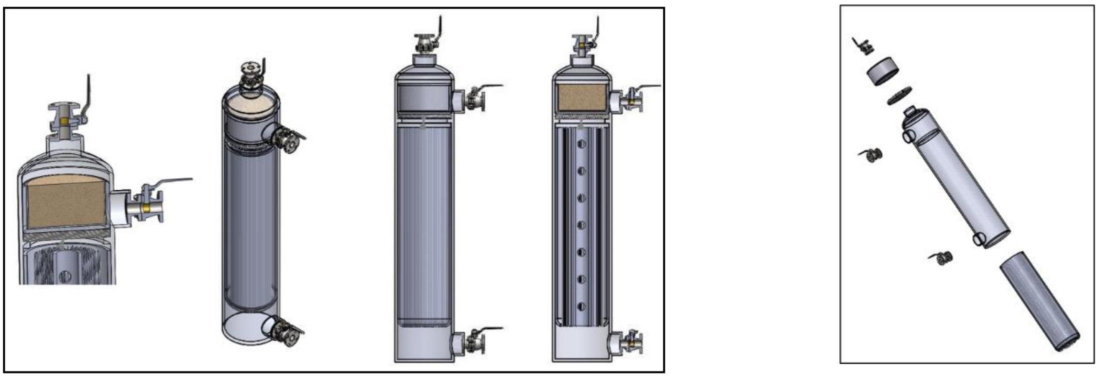
Fig. 8: Initial 2D Design of Assembly

2.2. SolidWorks

In the final phase of this study, SolidWorks was used for the preparation of 3D model. This is because SolidWorks allows for better 3D modeling and is more widely used in the industry. The engineering drawings was generated along with the model for all the components in the design. An animation was made for the exploded view which helps in visualization.

2.3. 3D Model

The final 3D model produced by SolidWorks is shown in Fig. 9 (a) and (b) below. From left to right, see in order: Close up of the sand filter, isometric view of the membrane assembly, side view, side cross-section view. Standard valves were used and labeled V-01, V-02, and V-02 from top to down. The valves are two-way.



(a) **(b)**

Fig. 9: 3D Model (a) Final SolidWorks 3D Model of Assembly, (b) SolidWorks 3D Model Exploded View of Assembly

2.4. Engineering Drawings

The Fig. 10 shows the engineering drawings for proposed membrane assembly and are according to the calculated membrane specifications detailed in section 3.4. The dimensions are in millimeters.

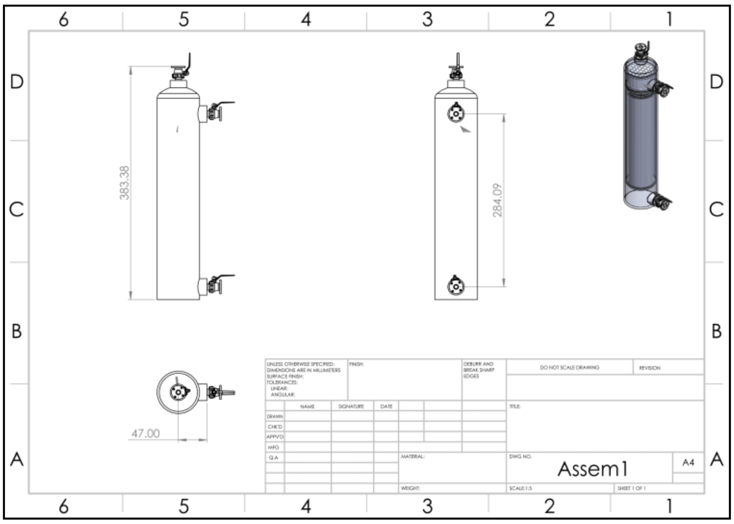


Fig. 10: Assembly Body Engineering Drawing

2.5. Removal of Pollutants

If water has high acidity or low mineral content, it can corrode pipes. If these pipes contain lead, they can enter drinking water. There is a partial reduction of lead with UF. With the addition of graphene oxide, the removal rate rises to over

90% [10]. This is due to the adsorption sites present on the GO flakes that selectively adsorb heavy metal ions including arsenic. The Table 1 to 3 below show findings.

Table 1: IESE Water Supply Turbidity Tests

Location (IESE)	Turbidity (NTU)	
1st Floor Washroom Tap	0.98	Standard Deviation: 0.037
	0.92	Mean: 0.93
	0.89	Variance: 0.0014
Environmental Chemistry Lab Tap	1.53	Standard Deviation: 0.046
	1.42	Mean: 1.46
	1.45	Variance: 0.0022
1st Floor Drinking Water Filter	1.31	Standard Deviation: 0.021
	1.33	Mean: 1.31
	1.28	Variance: 0.0004

Table 2: PCRWR and Master's Thesis Reports

Parameter	Result (Mean)	NEQS (Drinking Water)
Color / Odor	Transparent / None	None
pH	7.2	6.5-8.5
TDS (mg/L)	300	<1000
Conductivity (uS/cm)	604	-
Temperature (Celsius)	25.1	-
CFU/100ml	>23	Must not be detected
Free Chlorine (mg/L)	0.13*	0.2-0.5
Arsenic (ppb)	0.26*	<0.05
Lead (mg/L)	0.01*	<0.05

Table 3: PCRWR and CDA Reports

Parameter	Result (ppm)	Guidelines
Hardness	270	<500
Alkalinity	330	<100
Ca	90	<100
Mg	11	<50
HCO3	330	125-350
Cl	20	<250
Na	50	<200
K	1.1	<20
NO3	4	<3

2.6. Membrane Characteristics and Efficiency

The membrane surface area was calculated along with dimensions [18]. The dimensions were compared to those of the membrane without graphene enhancement for the same flowrate. The Fig. 11 to 13 below show the results.

With Optimum Graphene Enhancement	
Length (L)	9.456" (240.18 mm)
Diameter (D)	2.5" (63.5 mm)
Wet weight	<0.9lb
Hollow fiber external diameter	0.028" (0.72 mm)
Hollow fiber internal diameter	0.015" (0.38 mm)

Fig. 11: Surface Area Calculation

Membrane Surface Area Calculation

Product flow required	2-3 gpm 0.681 m3/hr 16.4 m3/d	*(Average kitchen faucet value)*
Average permeate flux	100 LMH	
Qa = SA x Flux SA = Qa / Flux		
Surface Area (SA)	0.164 m2 1.765 ft2	

Surface Area	0.164 m^2
Dimensions	Calculated using interpolation from manual created by *ami membranes*.

Fig. 12: Dimensions summary

Without Optimum Graphene Enhancement	
Length (L)	40″ (1016 mm)
Diameter (D)	4″ (101.6 mm)

Fig. 13: Dimensions without gaphene

The final membrane characteristics, specifications, and removal efficiencies for target pollutants are shown in the Fig. 14 and 15 as below.

Material	Polyether Sulfone (PES) + GO (0.5% by weight)
Flow configuration	Hollow fiber, outside/in operation, dense support Dead-end at low constant pressure
Concentrate recirculation	None
Chemical cleaning	If need be, with caustic soda, acid, and chlorine.
External diameter	0.028″ (0.72 mm)
Internal diameter	0.015″ (0.38 mm)
Pore size	0.01 um
Max TMP	2.5 bar
Max Backwash Pressure and flow	2.5 bar using permeate at 34 m^3/hr
pH range	2-11
Water retention*	57%
Average contact angle*	53 degrees
Flux*	100 LMH
Temperature range	1-40 degrees Celsius

Fig. 14: GO-MEM Characteristics

The removal efficiency for various water quality targets are shown on the graph to the right.

Huge improvements relative to pure ultrafiltration purification systems are observed.

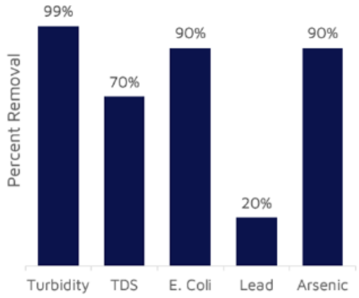


Fig. 15: Removal Efficiencies

3. Conclusion

The conclusions drawn from this study are that Flash Graphene is the most optimum current technology for the mass production of graphene. 0.5% by weight of graphene oxide is the most optimum amount of GO that should be added to PES membranes. PES membranes have large advantages over any other type of membrane. A large decrease in assembly size can be achieved (over 90%) by the addition of graphene oxide and flux is improved many folds up to 100 LMH. Over 99% turbidity removal and 90% bacterial and viral load reduction can be achieved from this membrane. Membrane life is up to 2 years and requires little to no maintenance in the form of backwashing. Hydrophilicity is also improved and makes this assembly a viable alternative to TWFs with similar costs.

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