

Simulation and Optimization Approaches for Productivity Improvement in Soft-Drink Industry Wastewater Management

Hifza Waseem

Department of Food Engineering
NED University of Engineering & Technology
Karachi, Pakistan
hifzawaseem6@gmail.com

Abstract

The study and proposed methodology address the pressing need for sustainable water management in industrial processes. Focusing on enhancing water recycling and reuse, particularly from bottle washer wastewater, our aim is to reduce resource consumption and operational costs associated with wastewater treatment while maintaining water productivity improvement. After conducting a comprehensive study on various treatment processes, we designed and implemented a Membrane Bioreactor (MBR) system. In the subsequent phase, we synthesized an antifouling Nano-filtration (NF) membrane to optimize filtration efficiency within the MBR. This involved thorough experimentation to assess numerous membrane parameters and simulation using COMSOL Multiphysics (the objective is to simulate various physical phenomena and properties of the membrane including fluid dynamics, mass transfer, thermal analysis to better understand its behavior and optimize its performance.) and Material Studio (primary aim is to simulate and assess material characteristics and behaviors at atomic and molecular scales such as molecular dynamics, quantum mechanics, crystal structure, and thermodynamics). Our findings suggest that the integration of this modified antifouling self-cleaning NF membrane offers a promising strategy for improving water treatment processes, reducing fouling, and ensuring consistent supply of clean water. To streamline operations, GPS-X was employed for full-scale plant design, ensuring efficient and reliable performance. The results showed effective COD, BOD, and TSS reduction, supporting reuse for bottle washing (enhances production efficiency up-to 40%), cooling towers, and irrigation. This paper demonstrates the industrial feasibility and sustainability of nanocomposite MBR systems.

Keywords

Waste Water Reuse, Membrane Bioreactor, Nano Filtration Membranes, Process Simulation and Optimization, Productivity Improvement.

1. Introduction

The soft drink industry discharges large quantities of wastewater, particularly from bottle washing processes. This untreated discharge contains surfactants, detergents, suspended solids, and pollutants (Rashid et al. 2021). Wastewater treatment removes and eliminates pollutants from wastewater. This process helps wastewater convert into an effluent that can be recycled to the water cycle (Gamri et al. 2022). However, according to a survey report, the bottle washing process consumes significant quantities of water, with modern washers using around 150 to 200 ml per bottle, accounting for approximately 50–60% of a plant's daily water usage (Bienati et al. 2008). Hence, an innovative treatment approaches, based on simulation and optimization tools, are necessary to improve reuse of wastewater and ensure sustainable soft drink production.

In soft drink production. The most water-intensive operation is the washing of regular glass bottles. The cleaning procedure enhances the water consumption and promotes discharge to the same extent. The effluent is rich in total

solids, which is difficult to recycle with conventional methods. Dependence on fresh consumption is not an efficient or viable option, especially when high costs halt operations and impact production.(Abd-Elaal 2021)

1.1 Objectives

The study covers the implementation of advanced alternatives that are based on simulation-driven approaches, which can evaluate treatment performance, optimize operating conditions, and support the design of full-scale plants. Such integrated strategies will not only enable wastewater reuse but also improve productivity and sustainability in beverage manufacturing.

Cost reduction is a crucial factor in sustainable practices. By optimizing wastewater treatment processes, such as utilizing innovative technologies or streamlining treatment methods, significantly decrease operational expenses. This aspect emphasizes not just the treatment and its cost but also the broader goal of resource conservation.

2. Literature Review

The treatment proceeded with three methods Primary, Secondary and Tertiary. Primary wastewater treatments are the first step that we use to treat wastewater to free it from solid particles by usually physical processes like sedimentations, filtration, distillation etc. After doing primary treatment now it is the time for secondary treatment. It is used to remove organic compounds from waste water using organic techniques such as bio-filtration, Aeration. Tertiary is the last stage of wastewater treatment. This is very important step as the water are supposed to be cleaned completely. The main purpose of this step is to remove pathogens like phosphate and nitrate from the wastewater.(Kuş and Kara 2025)

2.1 Membrane Filtration

A promising technology, has garnered global attention, especially with extensive research on poly ether sulfone (PES) membranes. PES, renowned for its thermal, chemical, and mechanical properties, finds applications in microfiltration (MF), ultrafiltration (UF), and nanofiltration (NF). However, PES's hydrophobic nature leads to membrane fouling, pore blocking, and biofouling. (Saniei et al. 2020)

To mitigate these issues, enhancing membrane hydrophilicity is essential. Incorporating hydrophilic materials, nanoparticles, and fillers into the membrane, particularly through nanoparticle embedment, has emerged as a key strategy. Researchers have explored various methods, such as adding functionalized additives, blending nanoparticles with the polymer matrix, and grafting modified membranes with additives, to improve self-cleaning properties and overall membrane performance. (Otitoju et al. 2020)

2.2 Membrane Bio Reactor

Conventional wastewater treatment methods face challenges like high energy consumption and limited efficiency, and they also struggle to remove certain contaminants fully and maintain consistent treatment performance. Conventional wastewater treatment plants also require a larger land space. These challenges lead to the adaptation of new advanced technologies like Membrane Bioreactor (MBR) which enhance the treatment efficiency, aiming to overcome limitations and promote sustainable wastewater management practices. (Chen et al. 2003)

The term membrane bioreactor (MBR) defines a combination of an activated sludge process and membrane separation into a single-step process. Unlike conventional methods, MBRs combine the advantages of biological treatment which facilitates the breakdown of organic contaminants. The key components of an MBR system include a biological reactor and a membrane filtration unit.(Goswami et al. 2018)

In the biological reactor, microorganisms break down organic pollutants in the wastewater through a biological process. The membrane filtration unit employs ultrafiltration or microfiltration membranes to separate treated water from suspended solids and microorganisms, providing a high-quality effluent. The biological process in the MBR converts dissolved organic matter into suspended biomass, reducing membrane fouling and allowing recovery to be increased.(Al-Asheh et al. 2021)

2.3 Membrane Characterization

Characterization of mixed matrix membranes (MMMs) is a crucial aspect of assessing their performance and understanding their suitability for specific applications.(Gallucci et al. 2011) Mixed matrix membranes combine both polymeric and inorganic components to exploit the synergistic effects of each material, aiming to enhance the overall

separation efficiency and mechanical properties. (Hadi Al Hasan 2019) The synthesized membranes underwent a thorough characterization, encompassing various analysis to elucidate their morphological structure, chemical composition, hydrophilicity, and surface roughness. (Xia et al. 2008).

3. Methodology

Membrane simulation is done by using Material Studio and COMSOL Multiphysics. We have two membrane polyether sulfones with Tannic acid, Tannic acid as nano particle while polyether sulfone considers as polymer. While Chitosan with zinc oxide, having Chitosan as polymer and zinc oxide as nano particle. Both simulated at Temperature: 25°C, 298k.

3.1 Membrane Forcite Dynamic Simulation

The Forcite Dynamic simulation within Material Studio provides an intricate analysis of the membrane's behavior at a molecular level. This simulation enables observation of how the membrane responds over time under varying conditions like pressure, temperature, and fluid composition. By monitoring these changes, insights into the membrane's structural integrity and stability under operational stresses can be gained. This dynamic simulation is pivotal for identifying potential weaknesses or failure-prone areas, guiding improvements in design for enhanced performance. Furthermore, it deepens understanding of how the membrane material interacts with permeating molecules, crucial for optimizing selectivity and permeability. Overall, Forcite Dynamic simulation plays a crucial role in predicting the membrane's long-term behavior and ensuring its reliability in practical applications

3.2 Forcite Geometric Optimization

Forcite Geometric Optimization is a critical process for refining membrane structure to achieve optimal performance. This method involves adjusting geometric parameters to enhance factors such as pore size distribution, surface area, and mechanical stability. Through iterative simulations and adjustments, this process balances trade-offs between different performance metrics to achieve better permeability, selectivity, and reduced fouling. The resulting optimized geometry extends the membrane's operational lifespan and enhances its efficiency, making it essential for membrane design and engineering.

3.3 Thermal Analysis

Thermal analysis plays a crucial role in characterizing membranes, as fluctuations in temperature can profoundly affect their performance and durability. Conducted using COMSOL, thermal analysis examines key properties such as thermal conductivity, heat capacity, and thermal expansion of the membrane material. Understanding these characteristics allows us to anticipate how the membrane will respond across different thermal environments. This analysis is instrumental in determining the ideal operating temperature range to maximize efficiency while preserving structural integrity. Moreover, thermal analysis identifies potential thermal stresses that could degrade the membrane over time. Addressing these insights enables the design of membranes with enhanced thermal stability, ensuring consistent and reliable performance in diverse real-world applications.

3.4 Fluid Interaction Analysis

Fluid interaction analysis in COMSOL is pivotal for optimizing membrane performance by visualizing flow dynamics and transport properties. Through fluid dynamics simulations, COMSOL illustrates velocity profiles, identifying areas of uniform flow and potential stagnation zones to optimize membrane designs for efficient fluid transport and reduced fouling. Species transport simulations assess solute movement via diffusion and convection, enhancing membrane configurations to improve separation efficiency and mitigate concentration polarization. Overall, these analyses in COMSOL contribute significantly to advancing membrane technology, ensuring membranes are tailored for diverse filtration and separation applications, maintaining reliability and efficiency across varying operational conditions.

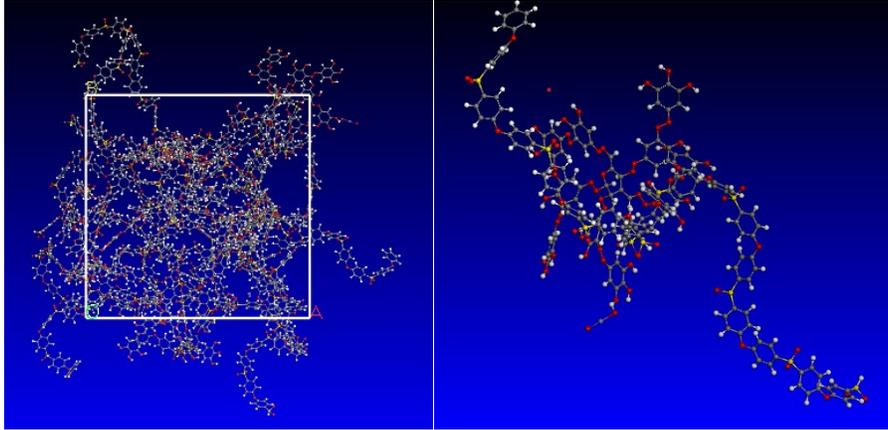


Figure 1. Membrane 1 PES with Tannic Acid

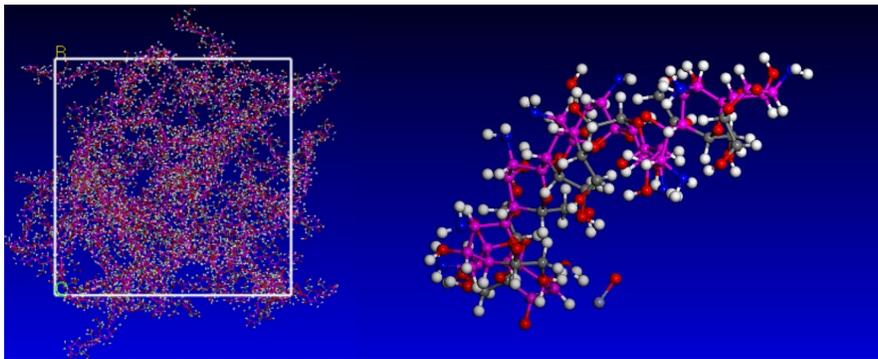


Figure 2. Membrane 2 Chitosan with Zinc Oxide

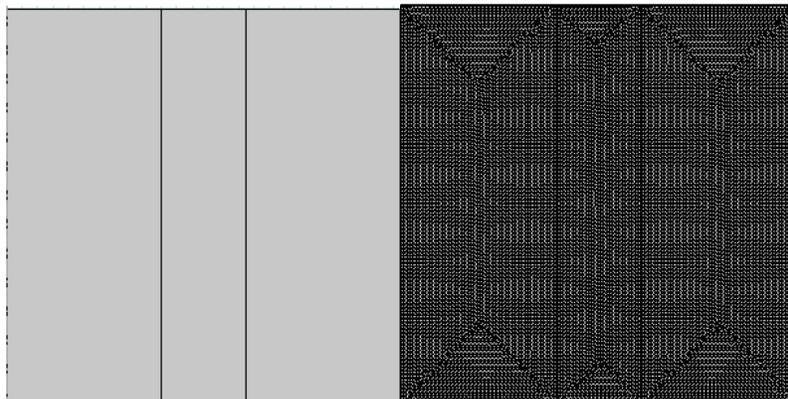


Figure 3. Physical Structure of Membrane

3.5 Plant Model

For Building plant layout following characteristics are followed

- Characterization of influent components
- The influent flowrate is set and control to 5000m³/day
- The given pH of influent is 11
- Set Volume of neutralization tank 850 m³
- Adjust MBR tank 4 tanks with total volume of 1000 m³
- Specifying pump efficiency set to 70%

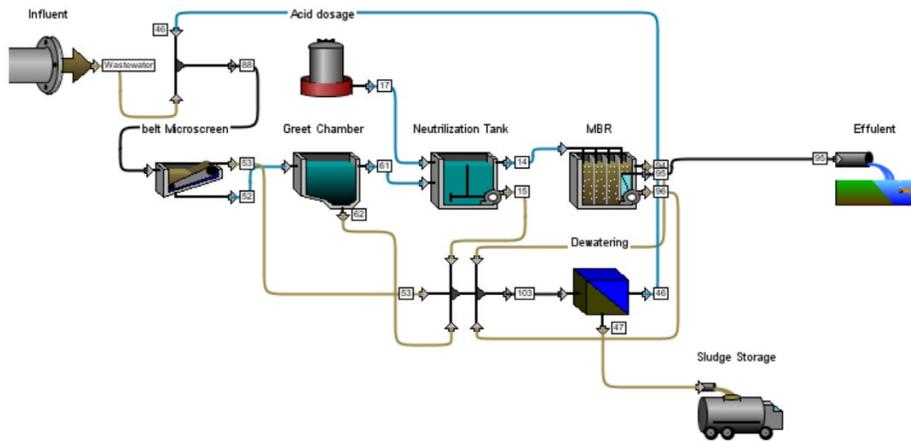


Figure 4. Model of Waste Water Treatment Plant based on MBR

4. Data Collection & Characteristic Identification

Length of membrane = 127mm

Width of membrane = 127 mm

Fluid aspect as (Table 1- Table 3)

Table 1. Parameters of Fluid

Parameter	Unit	Value
Initial concentration	mol/m ³	0
Final Concentration	mol/m ³	1200000
Velocity	m/s	5
Reference Temperature	k	298

Table 2. Characteristics of Bottle Wash Waste Water

Parameter	NEQS	Fresh Water Supplied	Bottle Wash Waste Water
pH	6.0-9.0	7.3	9 - 11
Turbidity (NTU)	-	2.5	12 - 25
TDS (mg/l)	3500	341	750 - 1200
TSS (mg/L)	200	-	26 - 90
COD (mg/L)	150	-	25 - 125
Hardness (mg/l)	-	51	125 - 150
Chloride (mg/l)	1000	-	412 - 615
Nitrate (mg/l)	-	2	3.0 - 15
Sulfate (mg/l)	600	51	112 - 280
Conductivity (µs/cm)	-	560	1050 - 3200

Table 3. Operational Parameters for Simulation

		Wastewater				
VSS/TSS Ratio	-	0.75				
		52				
Underflow as Fraction of Influent Flow	-	0.005				
		61				
Grit Production per Flow	mg/L	20.0				
Dry Solid Content of Grit	%	98.0				
		14				
Maximum Volume	m3	850.0				
Tank Depth	M	4.0				
Air Flow into Aeration Tank	m3/d	0.0				
		94(1)	94(2)	94(3)	94(4)	94
Surface Area in Final Tank	m2	-	-	-	-	40.0
Total Maximum Volume	m3	-	-	-	-	10000
Volume Fractions	-	0.25	0.25	0.25	0.25	0.25
Total Membrane Surface Area	m2	-	-	-	-	4000
Solids Capture Rate	-	-	-	-	-	0.9999
Colloidal Substrate Capture Rate	-	-	-	-	-	0.1
Soluble Inert Capture Rate	-	-	-	-	-	0.1
Air Flow into Aeration Tank	m3/d	-	-	-	-	20000
		46				
Removal Efficiency	-	0.95				
Removal Efficiency	-	0.95				

5. Results & Discussion

5.1 PES with Tannic Acid Membrane

The Simulation studies revealed that the incorporation of tannic acid with polyether sulfone improved the surface properties of the membrane. This modification enhanced hydrophobicity of the material, which is a critical factor of handling foulant deposition during waste water treatment. This structural moderation improves antifouling properties and increases stability and life span under high load of contamination (Table 4, Figure 5- Figure 8).

Table 4. Transport Properties of PES with Tannic Acid Membrane

Parameters	Value
Molecular Weight	4.217083e+003 amu
Cp	237.63687147 J/mol.K
Thermal Conductivity	0.20188488 J/Kms
Diffusion Coefficient	1.000e-9 m ² /s
Permeability of oxygen	12.01178590 Dow
Permeability of nitrogen	2.50827986 Dow
Permeability of carbon dioxide	43.65876077 Dow
Density	4.97099837 gm/cm ³

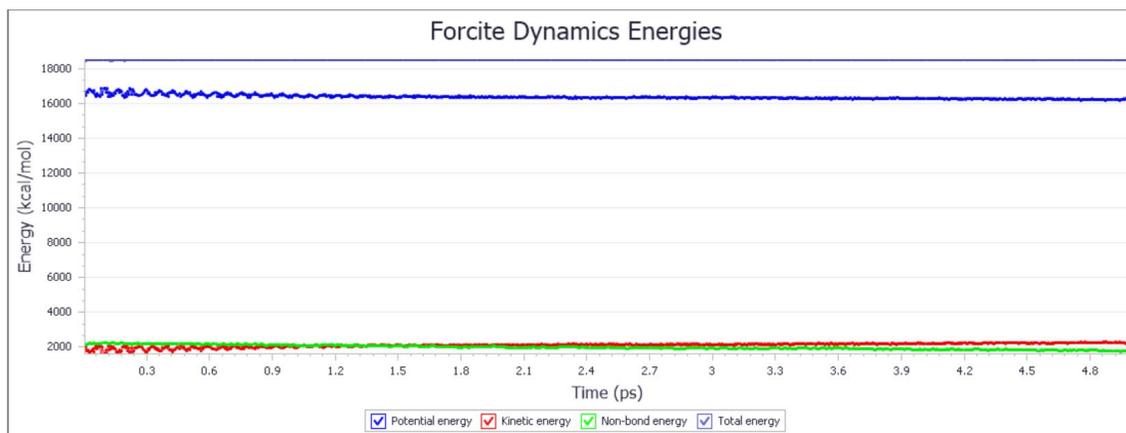


Figure 5. Forcite Dynamic trend of PES with Tannic Acid Membrane

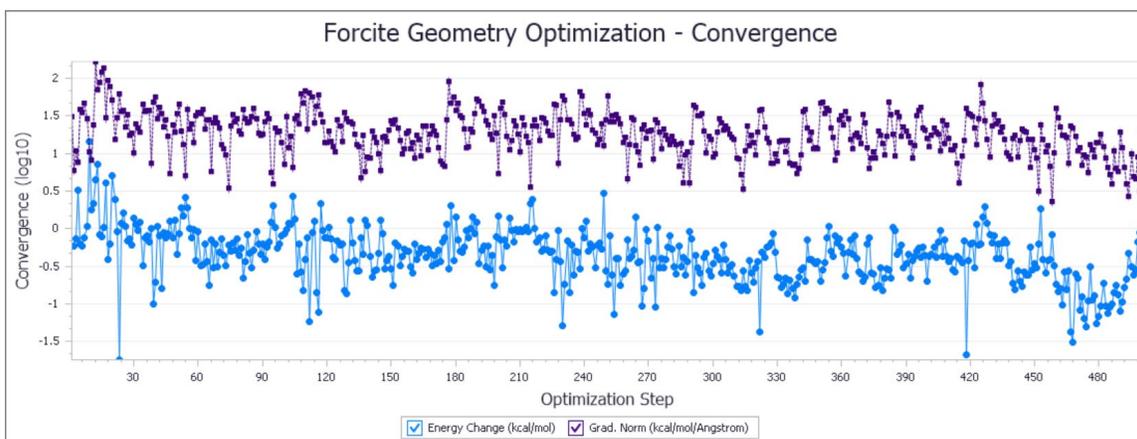


Figure 6. Forcite Geometry Optimization trend of PES with Tannic Acid Membrane

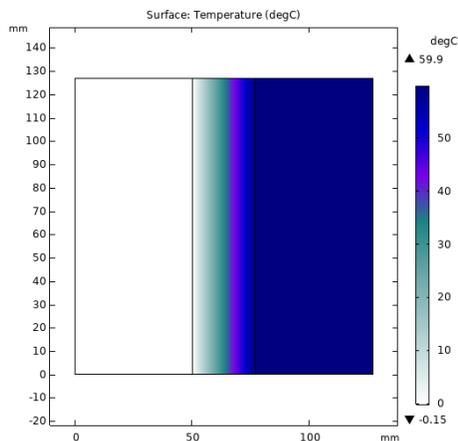


Figure 7. Thermal Analysis on surface of PES with Tannic Acid Membrane

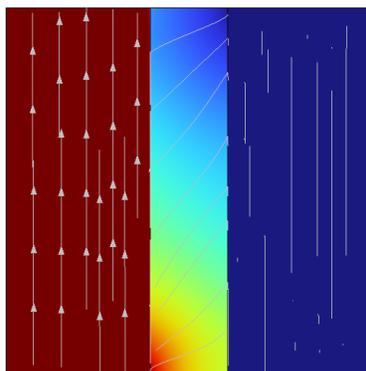


Figure 8. Fluid Interaction trend on surface of PES with Tannic Acid Membrane

5.2 Chitosan with Zinc Oxide Membrane

In chitosan-based membrane with zinc oxide nano particle exhibit the improvement in functional location. Zinc oxide enhanced surface activity with chitosan matrix increased it interaction with water molecule promoting better anti-bacterial and anti-fouling properties. Maintain high flux rate with low biofilm formation (Table 5, Figure 9- Figure 11).

Table 5. Transport Properties of chitosan with zinc oxide Membrane

Parameters	Value
Molecular Weight	5.390550e+004 amu
Cp	211.27577426 J/mol.K
Thermal Conductivity	0.20676680 J/Kms
Diffusion Coefficient	1.000e-5 m ³ /s
Permeability of oxygen	0.01244173 Dow
Permeability of nitrogen	0.00149560 Dow
Permeability of carbon dioxide	0.02448599 Dow
Density	1.44506392 gm/cm ³

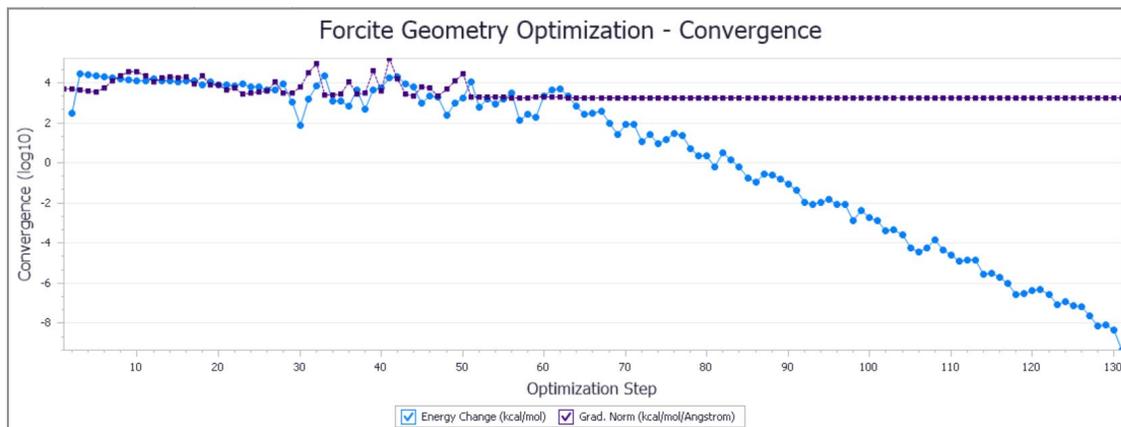


Figure 9. Forcite Geometry Analysis of Chitosan with Zinc Oxide Membrane

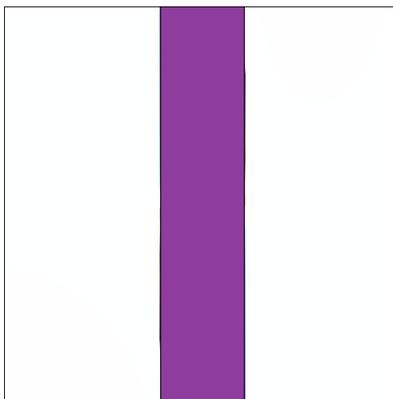


Figure 10. Thermal Analysis on the surface of Chitosan with Zinc Oxide Membrane

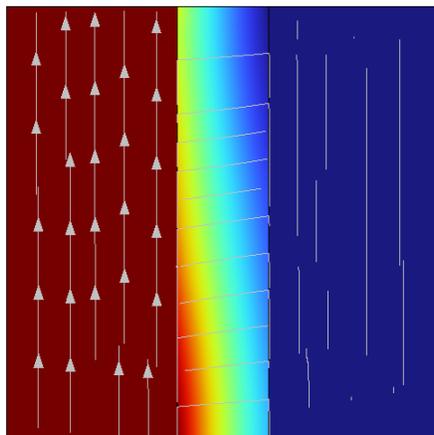


Figure 11. Fluid Interaction on the surface of Chitosan with Zinc Oxide Membrane

5.3 Effluent Outcome

The treated effluent water meets industry standards for cleaning glass bottles, with low solids and neutral pH, making it safe for use. Regular monitoring and maintenance are advised to ensure quality (Table 6 – Table 8, Figure 12)

Table 6. Simulation Result of Effluent

		95
Flow	m ³ /d	4256
TSS	mg/L	1.052
VSS	mg/L	0.4711
cBOD ₅	mg/L	0.9877
COD	mg/L	8.462
Ammonia N	mgN/L	3.596
Nitrite N	mgN/L	0.2081
Nitrate N	mgN/L	0.09183
TKN	mgN/L	4.51
TN	mgN/L	4.81
Soluble PO ₄ -P	mgP/L	0.2005
TP	mgP/L	0.3294
Total Alkalinity	mgCaCO ₃ /L	126.0
pH	-	7.0
DO	mgO ₂ /L	0.01798

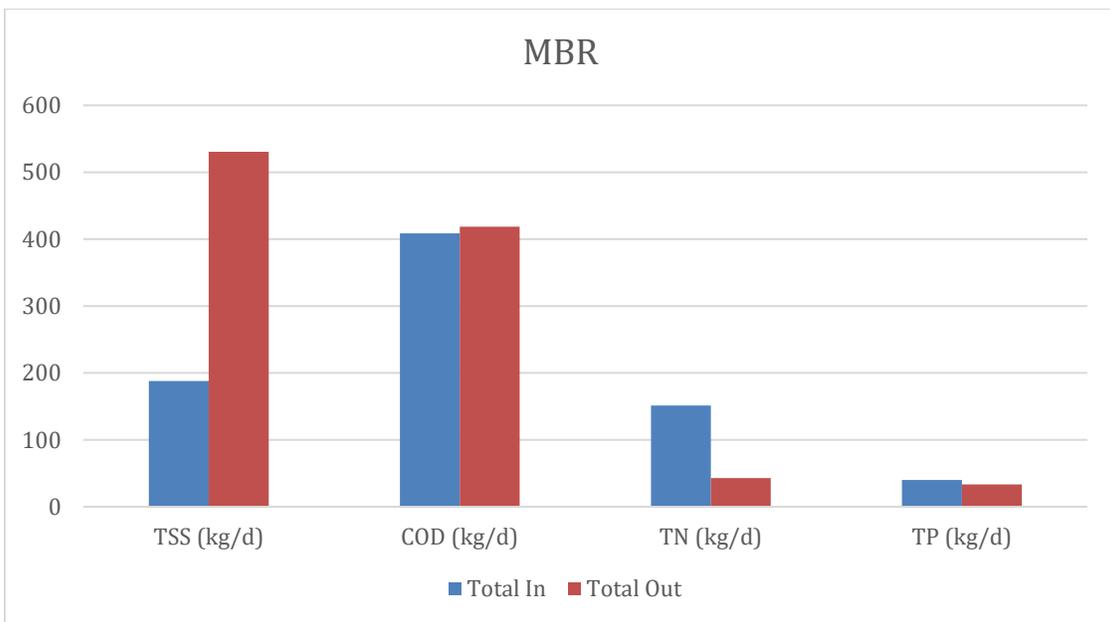


Figure 12. Total In and Out of Effluent

Table 7. Energy Consumption Summary of Plant

	Aeration Power (kW)	Pumping Power (kW)	Mixing Power (kW)	Heating Power (kW)	Other Power (kW)	Total Power (kW)
Influent (Wastewater)	0.00	1.36	0.00	0.00	0.00	1.36
Belt Microscreen	0.00	0.01	0.00	0.00	2.30	2.31
MBR	172.44	0.02	30.00	0.00	0.00	202.45
Dewatering	0.00	0.00	0.00	0.00	2.20	2.20
Layout Total	172.44	1.38	30	0	4.5	208.32

Table 8. Operating Cost Summary of the Plant

	Aeration Cost (Rs/kg)	Pumping Cost (Rs/kg)	Miscellaneous Cost (Rs/kg)	Chemical Dosage Cost (Rs/kg)	Sludge Disposal Cost (Rs/kg)	Total Cost (Rs/kg)
Influent (Wastewater)	0.00	0.18256	0.00	0.00	0.00	0.18256
belt Microscreen	0.00	0.00112	0.00	0.00	0.00	0.00112
MBR	23.1756	0.00224	0.00	0.00	0.00	23.17784
Dewatering	0.00	0.00	0.00	0.00	0.00	0.00
Sludge Storage	0.00	0.00	0.00	0.00	2.884	2.884
Layout Total	23.1756	0.18592	0.00	0.00	2.884	26.24552

6. Conclusion

This study was undertaken to address the pressing challenge of managing wastewater generated from bottle washing in the beverage industry. A Membrane Bioreactor (MBR) system was developed and tested with two different nanocomposite membranes to identify the most effective configuration for large-scale application. Using simulation platforms including Material Studio, COMSOL Multiphysics, and GPS-X, membrane formulations were evaluated to compare their structural stability, transport behavior, and treatment performance. The PES with tannic acid displayed enhanced anti-fouling properties and improved surface hydrophilicity, while retaining the mechanical and chemical stability. In parallel, chitosan membranes incorporated with zinc oxide nanoparticles demonstrated strong antibacterial activity and resistance to biofilm formation, supporting long-term operational performance. The findings providing the pathway to optimize waste water treatment and improved productivity by producing effluent with reduce COD, BOD, and TSS, producing water of sufficient quality for reuse in bottle washing, cooling systems, and irrigation. These outcomes highlighted that simulation-based optimization offers a practical route to reducing freshwater consumption, lowering treatment costs, and improving productivity in beverage manufacturing.

References

- Abd-Elaal, Alaa-Eldin M. “The Influence of Simultaneous Operation of Plumbing Appliances on Water Consumption and Conservation inside Residential Buildings.” *Ain Shams Engineering Journal* 12 (3): 2443–52. 2021.
- Al-Asheh, Sameer, Marzieh Bagheri, and Ahmed Aidan. “Membrane Bioreactor for Wastewater Treatment: A Review.” *Case Studies in Chemical and Environmental Engineering* 4 (December): 100109. 2021.
- Bienati, Barbara, Aldo Bottino, Gustavo Capannelli, and Antonio Comite. “Characterization and Performance of Different Types of Hollow Fibre Membranes in a Laboratory-Scale MBR for the Treatment of Industrial Wastewater.” *Desalination* 231 (1–3): 133–40. 1.2007.10.027. 2008.
- Chen, T.K., J.N. Chen, C.H. Ni, G.T. Lin, and C.Y. Chang. “Application of a Membrane Bioreactor System for Opto-Electronic Industrial Wastewater Treatment - a Pilot Study.” *Water Science and Technology* 48 (8): 195–202. 2003.
- Gallucci, Fausto, Angelo Basile, and Faisal Ibney Hai.. “Introduction – A Review of Membrane Reactors.” In *Membranes for Membrane Reactors*, 1st ed., edited by Angelo Basile and Fausto Gallucci. Wiley. 2011
- Gamri, Tarig El, Amir B Saeed, and Sara Sm Suliman. “Towards an Integrated Management of Treated Wastewater in Khartoum.” *Acta Scientific Agriculture*, June 1, 65–74. 2022.
- Goswami, Lalit, R. Vinoth Kumar, Siddhartha Narayan Borah, N. Arul Manikandan, Kannan Pakshirajan, and G. Pugazhenth. “Membrane Bioreactor and Integrated Membrane Bioreactor Systems for Micropollutant Removal from Wastewater: A Review.” *Journal of Water Process Engineering* 26 (December): 314–28. 2018.
- Hadi Al Hasan, Nuha. “Molecular Dynamic Simulation of the Density and Mechanical Properties of Polyvinyl Chloride(PVC)/High Density Polyethylene (HDPE) Composites Based on Materials Studio.” *Journal of Physics: Conference Series* 1294 (5): 052062. 2019.
- Kuş, Bayram Arda, and Tolgay Kara. “Advancements in Wastewater Treatment Systems: Integrating Simulation and Optimization for Improved Performance.” In *Wastewater Treatment Plants*, edited by Salah Souabi, Abdelkader Anouzla, Shalini Yadav, Vijay P. Singh, and Ram Narayan Yadava, vol. 130. Water Science and Technology Library. Springer Nature Switzerland. 2025.
- Otitoju, Tunmise Ayode, Mohsen Ahmadipour, Sanxi Li, Noor Fazliani Shoparwe, Liau Xin Jie, and Afolabi Lukmon Owolabi. “Influence of Nanoparticle Type on the Performance of Nanocomposite Membranes for Wastewater Treatment.” *Journal of Water Process Engineering* 36 (August): 101356. 2020.
- Rashid, Ruhma, Iqrash Shafiq, Parveen Akhter, Muhammad Javid Iqbal, and Murid Hussain. “A State-of-the-Art Review on Wastewater Treatment Techniques: The Effectiveness of Adsorption Method.” *Environmental Science and Pollution Research* 28 (8): 9050–66. 2021.
- Saniei, N., N. Ghasemi, A.A. Zinatizadeh, S. Zinadini, M. Ramezani, and A.A. Derakhshan. “Preparation and Characterization of a Novel Antifouling Nano Filtration Poly Ethersulfone (PES) Membrane by Embedding Goethite-Tannic Acid Nanoparticles.” *Separation and Purification Technology* 241 (June): 116646. 2020.
- Xia, Siqing, Jifeng Guo, and Rongchang Wang. “Performance of a Pilot-Scale Submerged Membrane Bioreactor (MBR) in Treating Bathing Wastewater.” *Bioresource Technology* 99. 2008.

Biography

Hifza Waseem is a recent graduate in Food Engineering from NED University of Engineering & Technology, Karachi. With a strong academic foundation and hands-on research experience, she has developed expertise in food product development, quality assurance, and innovative processing techniques. During her undergraduate studies, she actively engaged in research, including her final year project on wastewater treatment through membrane bioreactor technology, which she presented poster at the 1st International Conference of Food Engineering and the 3rd Sindh HEC Research Exhibition at Expo Centre Karachi.