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Machine Learning in Membrane Distillation for Pulp and Paper Wastewater Treatment: A Review

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ABSTRACT
Membrane distillation (MD) is a promising thermally driven separation technology for treating high-strength industrial wastewater, particularly from the pulp and paper industry. However, its performance is constrained by complex and nonlinear interactions among operating conditions, feed characteristics, and membrane properties, leading to challenges such as fouling, membrane wetting, and flux decline. Conventional modelling approaches are often inadequate in capturing these dynamic behaviours, resulting in limited predictive reliability. This review focuses on the application of machine learning (ML), with particular emphasis on artificial neural networks (ANNs), in enhancing MD performance prediction and optimization. ANN models have demonstrated strong capability in modelling nonlinear relationships and accurately predicting key performance indicators, including permeate flux, rejection efficiency, and fouling behaviour. Special attention is given to recent developments integrating ANN models with advanced membrane materials, such as polyvinylidene fluoride/cellulose nanocrystal (PVDF/CNC) composite membranes, to improve system efficiency and stability. Furthermore, probabilistic approaches, including Bayesian neural networks and Monte Carlo simulations, are discussed for uncertainty quantification and risk-informed decision-making. Key challenges, including data scarcity, model interpretability, and generalizability, are critically evaluated alongside emerging solutions such as explainable AI and digital twin systems. Overall, ANN-driven approaches offer significant potential to transform MD into a predictive, reliable, and intelligent wastewater treatment technology.

Keywords: Artificial Neural Networks (ANN), Membrane Distillation (MD), Pulp and Paper Wastewater, Machine Learning (ML), Fouling Prediction

1.0 INTRODUCTION

It has been established that the pulp and paper industry is among the largest consumers of freshwater resources and one of the main sources of wastewater in industries due to high

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consumption of water during various steps of pulp and paper manufacturing. On a global scale, this industry produces some of the highest volumes of wastewater where up to 60 m^3 of wastewater can be produced per each ton of paper products. Moreover, pulp and paper wastewater is characterized by high pollutant loadings, with Chemical Oxygen Demand (COD) typically ranging from 1,000–5,000 mg/L, Biological Oxygen Demand (BOD) between 500–3,000 mg/L, and Total Dissolved Solids (TDS) exceeding 2,000 mg/L, depending on the production stage. These high concentrations, along with the presence of lignin, chlorinated organics, and recalcitrant compounds, make treatment particularly challenging [1, 2]. These characteristics, combined with large discharge volumes, pose significant environmental risks and create challenges for effective wastewater management.

The complexity of pulp and paper wastewater arises from multiple stages of the production process, including raw material preparation, pulping, bleaching, and finishing. Each stage generates distinct pollutants, resulting in highly variable and heterogeneous effluent compositions. As summarized in Table 1, wastewater streams may contain suspended solids, phenolic compounds, lignin, volatile organic compounds, chlorinated derivatives, dyes, and non-biodegradable additives, all of which contribute to treatment difficulty and increase the complexity of wastewater treatment processes [1,2]. In addition, the distribution of wastewater generation points across the production cycle is illustrated in Figure 1, highlighting the multiple sources and variability of pollutants within the system. This variability reduces the effectiveness of conventional biological and physicochemical treatment processes, particularly for removing recalcitrant compounds such as lignin and color-causing substances.

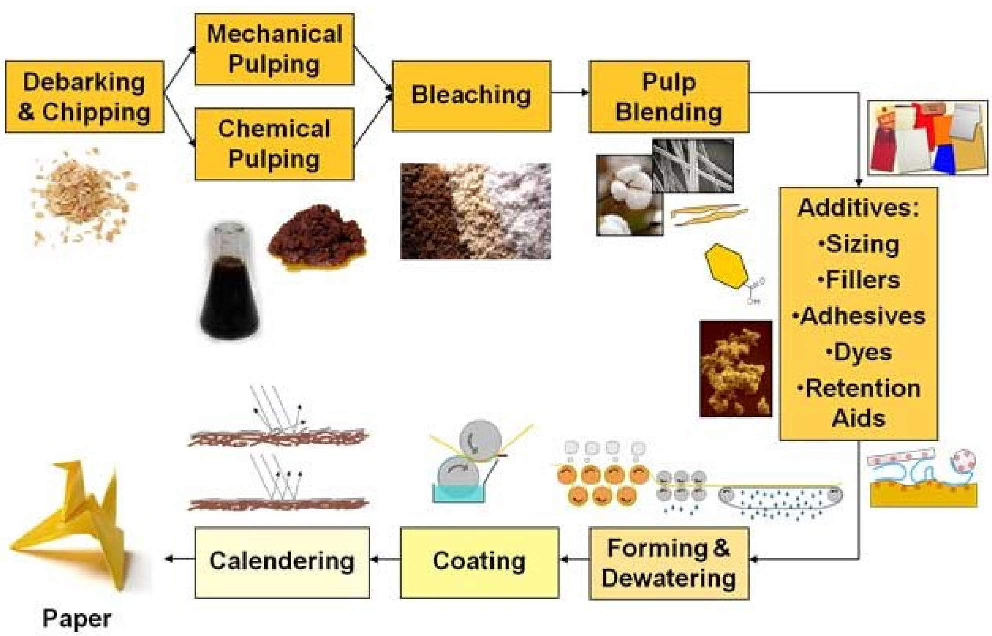

Figure 1. Stages of pulp and paper production and associated wastewater generation points. [3]

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Table 1. Pollutant generating processes at different stages of paper making

Stage of Process	Pollutant Sources / Activities	Major Pollutants	Treatment Challenges	References
Raw Material Preparation	Debarking, wood chipping	Suspended solids, bark, tannins, phenols	High particulate load; low biodegradability of phenolics	[2,4]
Chemical Pulping	Cooking with $NaOH/Na_2S$; black liquor	Lignin, volatile organics, sulphur compounds, high COD/BOD	High organic load; strong odour; requires complex biological or oxidation processes	[1,2,5]
Mechanical Pulping	Grinding, refining with minimal chemicals	Fibers, extractives, high BOD	Large volume, dilute but biologically active effluent	[2,4]
Bleaching	Chlorine, chlorine dioxide, oxygen, peroxide	Chlorinated organics, adsorbable organic halides (AOX), dioxins, colour	High toxicity; persistent organic pollutants; difficult to degrade	[1,2,5]
Papermaking and Finishing	Sizing, dyeing, coating, starch use	Dyes, starch, biocides, synthetic resins, high COD and colour	Variable wastewater composition; presence of non-biodegradable compounds	[1,2,4,6]

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These problems can be overcome using integrated wastewater treatment technologies incorporating anaerobic digestion, aerobic treatment, and advanced oxidation process (AOP). The structure of one such system is shown in Figure 2 [3] with anaerobic digestion serving to reduce organic content and recover energy, while aerobic treatment serves to further break down the organic pollutants. The AOP stage is generally applied as the final stage for the removal of persistent organics from the water body. Despite these advancements, conventional treatments still struggle to achieve complete removal of complex pollutants, especially under fluctuating wastewater conditions [1, 2, 5].

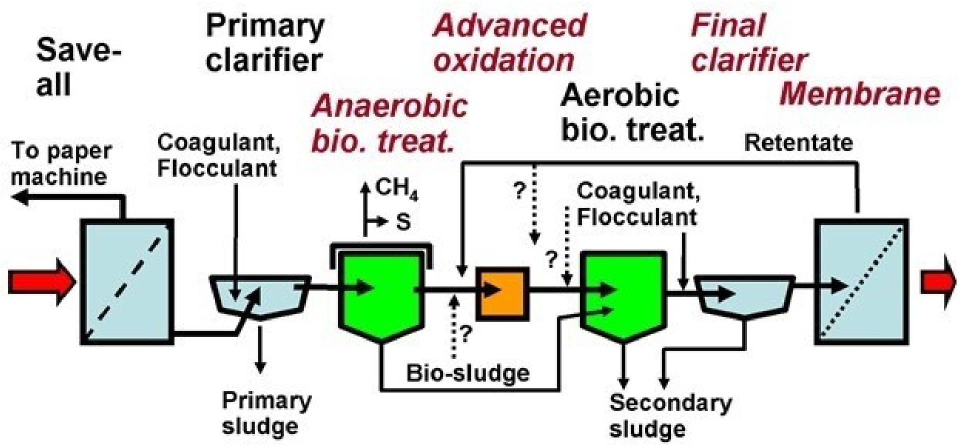

Figure 2. Schematic diagram showing options for enhancements of wastewater treatment plants for the pulp and paper industry [3]

As shown in Table 2, membrane-based technologies such as microfiltration (MF), ultrafiltration (UF), nanofiltration (NF), and reverse osmosis (RO) have been widely investigated for pulp and paper wastewater treatment due to their high separation efficiency. However, these pressure-driven processes often suffer from severe fouling and high energy consumption, particularly under high salinity and organic loading conditions [4,6]. Membrane distillation (MD) has emerged as a promising alternative owing to its ability to achieve near-complete rejection of non-volatile contaminants while utilizing low-grade or waste heat. Therefore, this review focuses on MD as a viable advanced treatment technology and explores how machine learning can enhance its prediction, optimization, and operational reliability [7,8]. This unique mechanism enables MD to achieve near-complete rejection of salts and organic pollutants while utilizing low-grade or waste heat, making it particularly suitable for high-temperature and high-salinity industrial wastewater.

Applications of membrane distillation (MD) across various industrial sectors are presented in Table 3, demonstrating its effectiveness in treating challenging effluents with high organic content and salinity. However, despite its advantages and strong potential, MD still faces key challenges for practical implementation, including membrane fouling, pore wetting caused by surfactants, flux decline, and low thermal efficiency [9,10]. These limitations are largely influenced by the properties of the membrane materials. Table 4 summarizes commonly used MD membrane materials PVDF, PP, and PTFE with respect to their hydrophilicity, fouling resistance, thermal stability, and overall performance. Although PVDF membranes are widely favored due to their tunable properties, achieving stable long-term operation remains a challenge.

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Table 2. Overview of membrane technologies commonly used in wastewater treatment

Technology	Pore Size	Driving Force	Typical Materials	Pollutants Removal Targets	Flux (LMH)	Rejection (%)	Energy Consumption	Fouling Tendency	References
MF	0.1–10 µm	Hydrostatic pressure (0.1–0.5 bar)	PSf, PVDF, PES, PAN, PVA, PVC	Suspended solids, fibers, fillers	50–200	~0–20	Low	High (particulate fouling)	[6,11,12]
UF	1–100 nm	Pressure (1–3 bar)	PSf, PVDF, PES, PAN, chitosan	Macromolecules, lignin, colloids	20–150	60–90	Low–Moderate	Moderate–High	[6,11,13]
NF	~1 nm (200–1000 Da)	Pressure (4–10 bar)	Polyamide (TFC), PSf, PVDF	Divalent salts, color, small organics	10–50	80–95	Moderate	High	[11,12,13]
RO	<0.5 nm (<200 Da)	High pressure (10–40 bar)	Polyamide (TFC), PVDF	Salts, organics, micropollutants	10–40	>95–99	High	Very high (scaling & fouling)	[11,12,13]
MD	0.1–1 µm	Temperature gradient (non-isothermal)	PP, PVDF, PTFE, modified PVDF (e.g., CNC, TiO_2)	Non-volatile solutes, salts, organics	5–30	~99–100 (non-volatile)	Moderate–High (thermal)	Moderate (wetting + fouling)	[9,14,15]

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While advancements in membrane materials and process configurations have contributed to improving MD performance, challenges related to system predictability, process optimization, and operational reliability persist. Conventional mechanistic models often fail to capture the complex and nonlinear interactions between operating conditions, membrane characteristics, and highly variable wastewater composition. This limitation is particularly evident in modelling fouling behaviour and system dynamics under real industrial conditions [16,17].

Compared with other industrial wastewater streams, pulp and paper wastewater contain complex organic pollutants, including lignin, resin acids, dyes, chlorinated compounds, and surfactants, which substantially influence membrane fouling, pore wetting, and overall MD performance [1,2]. These constituents exhibit highly variable concentrations depending on the pulping, bleaching, and papermaking processes, resulting in complex interactions that are often difficult to capture using conventional mechanistic models. Consequently, in addition to traditional MD operating parameters such as feed temperature, feed flow rate, salinity, and membrane characteristics, wastewater-specific variables including lignin concentration, organic composition, color intensity, COD, TDS, and surfactant concentration should be incorporated into machine learning (ML) models to improve prediction accuracy and process understanding [1, 2].

Recent advances have demonstrated the potential of ML techniques, particularly Artificial Neural Networks (ANN), Support Vector Machines (SVM), and Random Forest (RF), for predicting key MD performance indicators such as permeate flux, rejection efficiency, and membrane fouling behavior. ANN models are particularly effective in capturing the nonlinear relationships between feed characteristics, operating conditions, and system performance, enabling accurate prediction of flux decline and fouling progression. Similarly, RF models have been employed to identify dominant fouling-related variables and evaluate the relative importance of process parameters, while SVM models have shown strong predictive capability when working with limited datasets. Compared with traditional empirical correlations, these data-driven approaches offer superior predictive accuracy, robustness, and adaptability, making them promising tools for the optimization and intelligent operation of MD systems treating complex wastewater such as pulp and paper effluent [18, 19, 20, 21]

Therefore, the novelty of this review lies in its focus on the potential application of ML in MD systems for pulp and paper wastewater treatment. While typical reviews may highlight membrane materials or MD processes development, this review emphasizes the importance of ML techniques as a tool in predicting the performance, optimizing, and assessing uncertainties in the treatment process.

2.0 OVERVIEW OF MEMBRANE DISTILLATION AND ITS CHALLENGES

MD as an equilibrium-based and thermally driven separation process, has gained attention for treating complex industrial wastewater such as that generated from pulp and paper operations [9,10,14]. This industry produces a diverse range of effluent types such as black liquor from the pulping process, effluents from bleach plants which contain halogenated organics, and finally, condensate wastewater, which contains volatile and dissolved organics. The characteristics of these effluents are diverse regarding their pH,

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temperature, and fouling potential due to the presence of lignin, hemicellulose breakdown products, resin acids, particulates, and surface-active substances [1,2,4].

Several MD processes have been examined for removing pollutants from industrial wastewater, with varying efficiencies and benefits related to their flux rates and thermal efficiencies. The basic process of MD, which uses vapor pressure gradient through a hydrophobic membrane [9,14], with volatile materials passing through the membrane and nonvolatile impurities staying behind. Among the different configurations, DCMD is the most common process since it involves a simple configuration with moderate permeate flux rates. AGMD incorporates an air layer into the process to minimize heat losses, thus making it more efficient thermally; however, the process becomes less efficient in flux [22,23]. VMD increases mass transfer by using vacuum on the permeate side, although system operation is quite complex [23]. MD configuration selection involves optimization between efficiency, energy usage, and feed properties, especially high temperature and salinity feeds. The DCMD configuration can be seen in Figure 3, where both the hot feed and cold permeate fluids meet either side of the membrane directly. The advantage of this configuration includes immediate condensation of the formed vapor inside the permeate stream, resulting in simplicity and efficient flux production. However, its major disadvantage lies in high conductive heat loss in the membrane [9, 22].

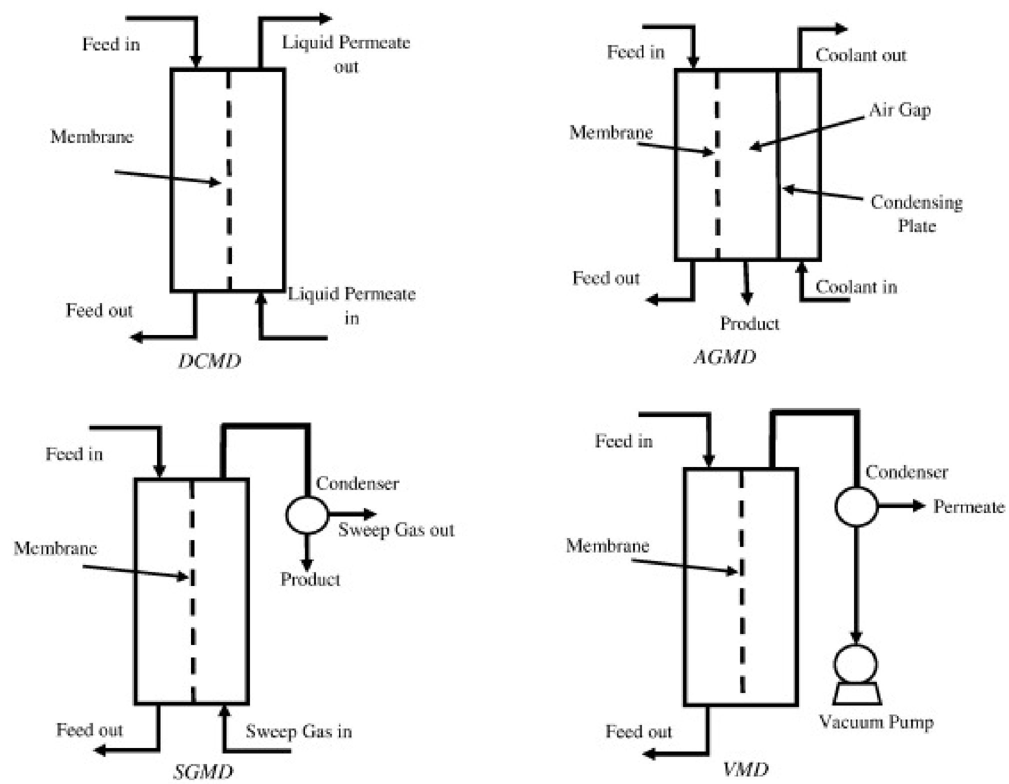

Figure 3. Schematic diagrams for the different types of MD configurations [24]

Applications of MD in different industrial applications are described in Table 3 and show its successful application in the treatment of difficult effluents with high organic loading and salinity. Nevertheless, despite all the advantages and prospects, MD faces significant problems in terms of practical realization, namely membrane fouling, pore

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wetting by surfactants, decrease in flux, and low thermal efficiency [9,14]. In turn, all these disadvantages are strongly dependent on membrane material properties, which are discussed in Table 4, where materials most often used for MD membranes Polyvinylidene fluoride (PVDF), polypropylene (PP), and polytetrafluoroethylene (PTFE) were considered regarding their hydrophilicity/fouling resistance/thermal stability/performance properties. Despite the popularity of the PVDF membranes due to its tunable properties, stable operation is still an unsolved issue.

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Table 3. Membrane distillation applications in industrial wastewater treatment

Industry	Wastewater Characteristics	MD Configuration	Membrane Material	Findings	Reference
Tissue Production	Moderate COD, TDS, resins, suspended solids; warm effluent	DCMD	PVDF flat sheet	>95% TDS removal, reduced turbidity, compatible with waste heat, suitable for water reuse	[24]
Cotton Fiber Bleaching	High pH, hydrogen peroxide, sodium hydroxide, high COD	VMD	PTFE hollow fiber	92% COD reduction, effective pH neutralization, minimal membrane fouling	[9]
Textile Dyeing & Finishing	High color, salts, surfactants, non-biodegradable dyes	DCMD	PP flat sheet	>98% color removal, excellent dye rejection, salt retention, potential for ZLD	[9]
Chemical Wastewater	High ammonia concentration, heat-intensive effluent	DCMD / VMD	PTFE flat sheet	Nearly 100% ammonia rejection, clean water recovery from volatile-rich streams	[9,14]
General Industrial	Salts, organics, surfactants, volatile organics	DCMD / AGMD / VMD	PVDF, PTFE, or modified PVDF	High rejection of non-volatiles, compatibility with high salinity, opportunities for ZLD	[9,10,14]

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Table 4. Comprehensive comparison of membrane materials, characteristics, and their impact on MD performance

Property/ Characteristic	PVDF (Polyvinylidene Fluoride)	PP (Polypropylene)	PTFE (Polytetrafluoroethylene)
Hydrophobicity	High; can be enhanced via modification	High	Very high; intrinsic property
Pore Size Range	10 nm – 1 µm (controllable)	0.1–1 µm	0.1–1 µm
Porosity	High (≥70%)	Moderate–High	High
Tortuosity	Moderate	Moderate–High	Low (favorable for flux)
Thickness	Thin (via phase inversion, NIPS)	Moderate	Moderate
Thermal Conductivity	Low	Low	Very low
Thermal Stability (°C)	~140–160	~100–120	~260
Chemical Resistance	Good	Moderate to good	Excellent
Mechanical Strength	High	Moderate	High
Fouling Resistance	Moderate (improved via CNC, TiO_2)	Moderate	High
Wetting Resistance	Moderate	Moderate	Excellent
Ease of Fabrication	Easy (phase inversion)	Easy (melt extrusion)	Difficult (sintering/stretching)
Cost	Moderate	Low	High
Pore Size Control	Good	Moderate	Difficult
Operational Lifespan	Moderate–High	Moderate	High
Typical Flux Range (LMH)	10–40	5–25	15–45
Rejection (%)	~99–100 (non-volatile solutes)	~98–100	~99–100
Application Suitability	Widely used in MD, UF, MF; highly modifiable	Mainly MF / support layers	Ideal for MD under harsh conditions
Research Trends	Most widely studied; strong focus on nanocomposite membranes (CNC, TiO_2, SiO_2)	Limited MD application; mostly support role	Moderate research; focused on durability and anti-wetting
Key Findings	Balanced performance, high tunability, improved antifouling via modification; best candidate for MD research	Economical but limited MD performance without modification	Superior hydrophobicity and resistance; best anti-wetting but costly and less scalable
References	[9,25,26]	[9,27]	[9,10,28]

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Despite its advantages, the potential of MD application in pulp and paper wastewater treatment is constrained by several critical operational bottlenecks. As can be seen from Table 3, membrane fouling is one of the major operational challenges in MD, particularly when treating pulp and paper wastewater due to the presence of lignin, resin acids, wood extractives, and other complex organic compounds that promote foulant deposition and flux decline [1,4,15,29]. The process of fouling occurs in different ways and includes organic fouling caused by the deposition of hydrophobic substances, inorganic fouling resulting from the presence of dissolved salts, and biological fouling associated with microorganism development. In addition to fouling, another crucial factor that restricts the use of MD technology is membrane wetting due to the presence of surfactants and other materials that lower surface tension and hydrophobic properties of the membrane and make it wet [10,15,29].

Therefore, while MD demonstrates strong potential for treating high-organic load wastewater, particularly in pulp and paper applications, overcoming these operational challenges remains essential. Dealing with fouling, wetting, and degradation in performance is vital in enhancing the reliability of the technology, which is an additional driver for utilizing ML modeling in MD systems.

3.0 OVERVIEW OF MACHINE LEARNING FRAMEWORKS IN MEMBRANE DISTILLATION

3.1 Data Acquisition and Preprocessing

The performance of ML algorithms on MD processes is largely determined by the suitability and representativeness of the datasets used in training the algorithm. Data for MD can generally be obtained from two major sources; experimental data collected from actual physical MD setups, and simulation data obtained through mathematical or thermodynamic modeling of the MD process. Experimental datasets provide realistic system behaviour but are often limited in size due to time and cost constraints. In contrast, simulated datasets offer flexibility and scalability, although they may not fully capture the complexity of real wastewater conditions [16, 17].

Data preprocessing is an important step in enhancing model performance and prediction accuracy. Data preprocessing includes feature selection, data normalization, and data cleansing. The important input variables that can be considered when building MD models include the temperature of the feed solution, feed flow rate, feed salt concentration, membrane characteristics (such as porosity and thickness), and operating conditions like pressure and recovery rate. All these variables play an important role in determining model outputs, including permeate flux, rejection ratio, and fouling tendency. Feature selection techniques are often employed to identify the most influential variables and reduce model complexity, while normalization ensures that all input variables are scaled consistently to improve convergence during training.

For pulp and paper wastewater applications, ML model development requires consideration of several wastewater-specific parameters. Besides conventional MD operating conditions such as feed temperature, flow rate, salinity, and membrane characteristics, additional parameters including COD, BOD, TDS, lignin concentration, color, pH, and conductivity significantly influence permeate flux, rejection performance,

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and membrane fouling. Therefore, feature-selection approaches are essential to identify the most influential variables and improve model robustness [21, 30].

3.2 Artificial Neural Networks (ANN) for MD Modelling

Several ML algorithms have been utilized in MD systems to model non-linear interactions and enhance prediction accuracy. In regression and prediction problems, ANN, SVM, RF, and LSTM neural network models are often used. One of the ML algorithms that are commonly employed in modeling MD systems is ANN models owing to their capability to discover complex non-linear relationships among process variables. As shown in Figure 4, the ANN model comprises three layers, namely input, hidden, and output layers connected by weights [16, 31]. Several studies have reported that ANN models outperform conventional empirical and regression-based approaches in predicting MD performance owing to their ability to account for complex interactions among multiple process parameters [21].

Despite their advantages, ANN models exhibit several limitations. The models generally require large and representative datasets for training, and their prediction performance may decline when applied to operating conditions beyond the training range. Furthermore, ANN models are often criticized for their limited interpretability, commonly referred to as the "black box" problem, where relationships between inputs and outputs are difficult to explain physically [18]. Nevertheless, ANN remains one of the most promising tools for MD performance prediction and optimization. Through this structure, ANN models can easily discover complex interaction among process parameters and performance. The ANN models exhibit better prediction results on permeate flux and thermal efficiency than the conventional empirical methods.

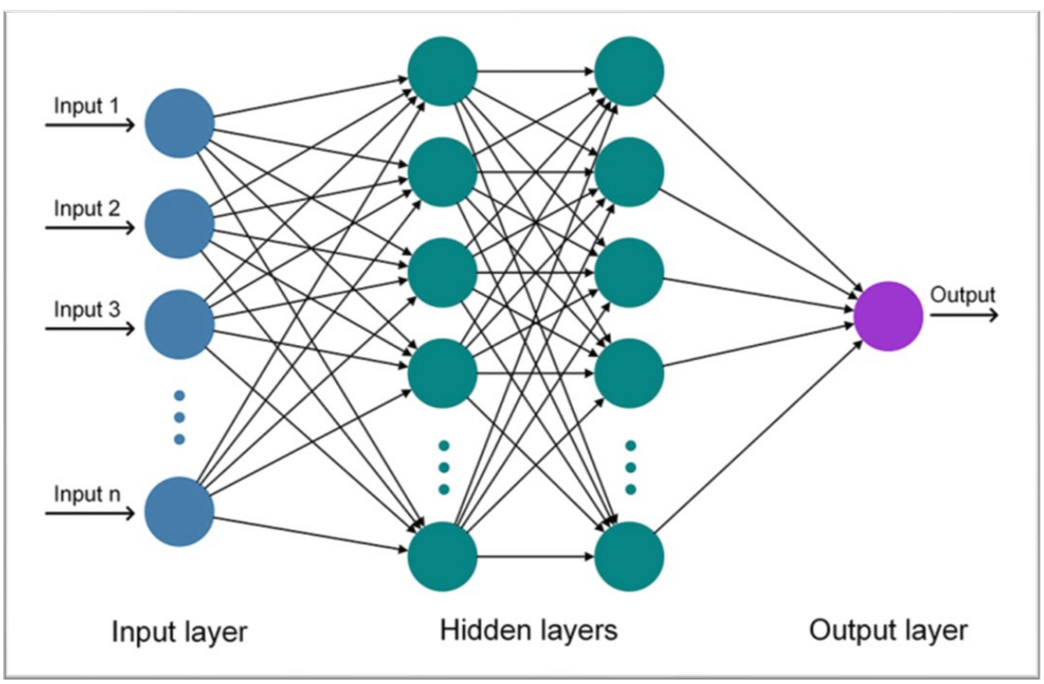

Figure 4. Schematic diagram of an Artificial Neural Network (ANN) [28]

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3.3 Support Vector Machine (SVM) and Ensemble Learning Approaches

In addition to ANN, support Vector Machine (SVM) as shown in Figure 5 is very efficient in small and high-dimensional datasets. The SVM ensures robust generalization through maximal separation of the points and has shown positive results in prediction of MD performance based on different operational conditions [25]. Using kernel functions, SVM can establish nonlinear decision boundaries and effectively model complex process behavior even when limited training data are available [32].

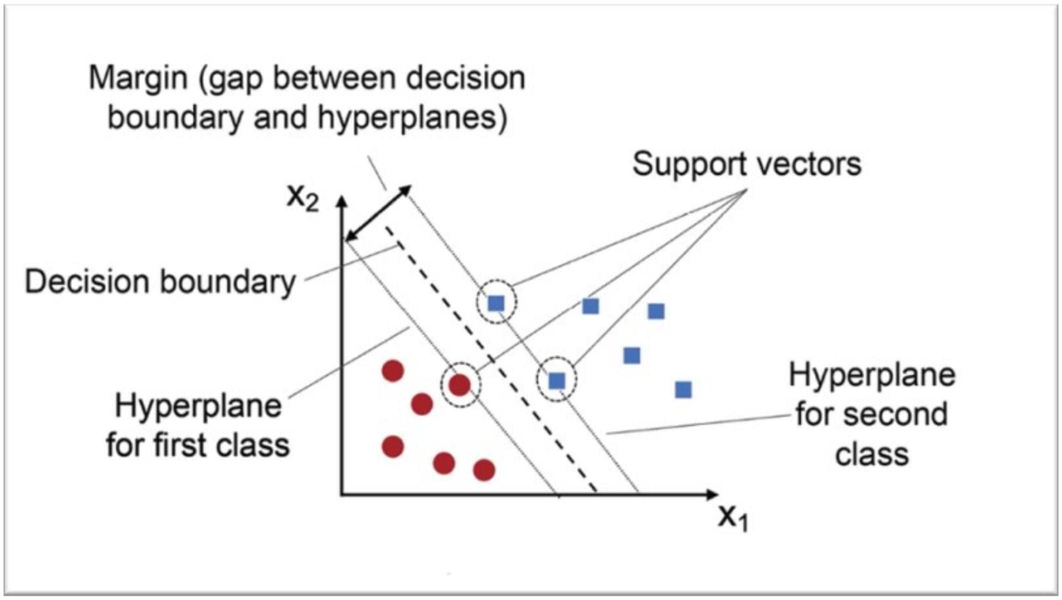

Figure 5. Schematic diagram of Support Vector Machine (SVM) [29]

Other ensemble algorithms like Random Forest (RF) and Gradient Boosting Machine (GBM) increase the efficiency of prediction by using several decision trees. As illustrated in Figures 6 and 7, enhance prediction performance through the integration of multiple decision trees. RF algorithm is used successfully for predicting fouling patterns and operational parameters that affect the performance of MD systems [33]. In contrast, GBM sequentially develops decision trees by focusing on correcting errors generated by preceding models, resulting in improved predictive accuracy [21].

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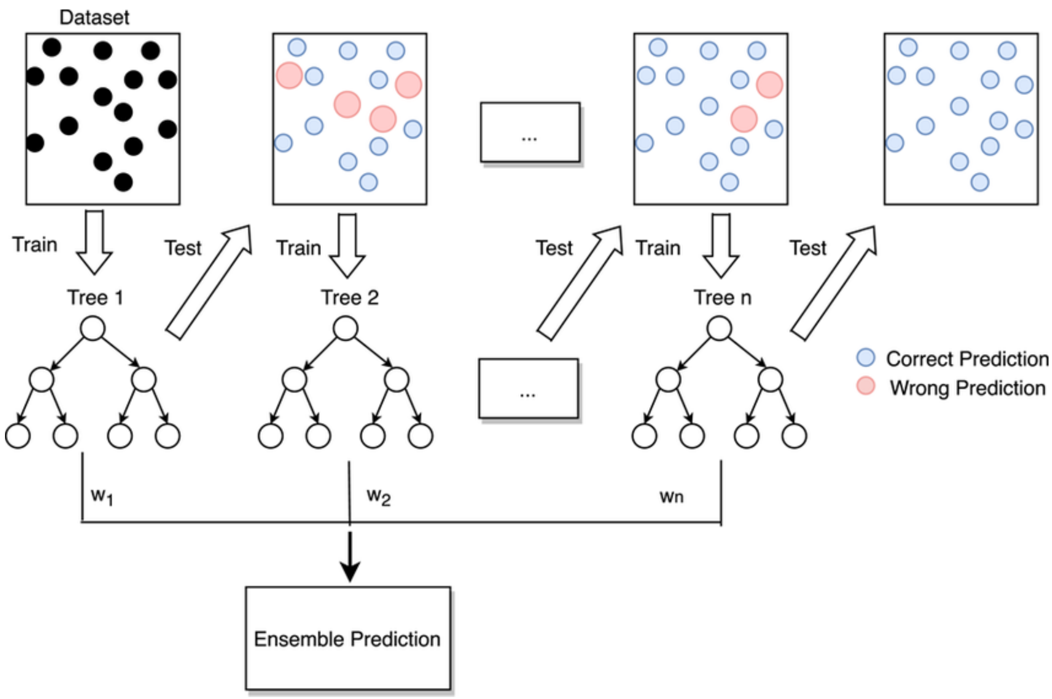

Figure 6. Schematic diagram of Gradient Boosting Machines (GBMs) [32]

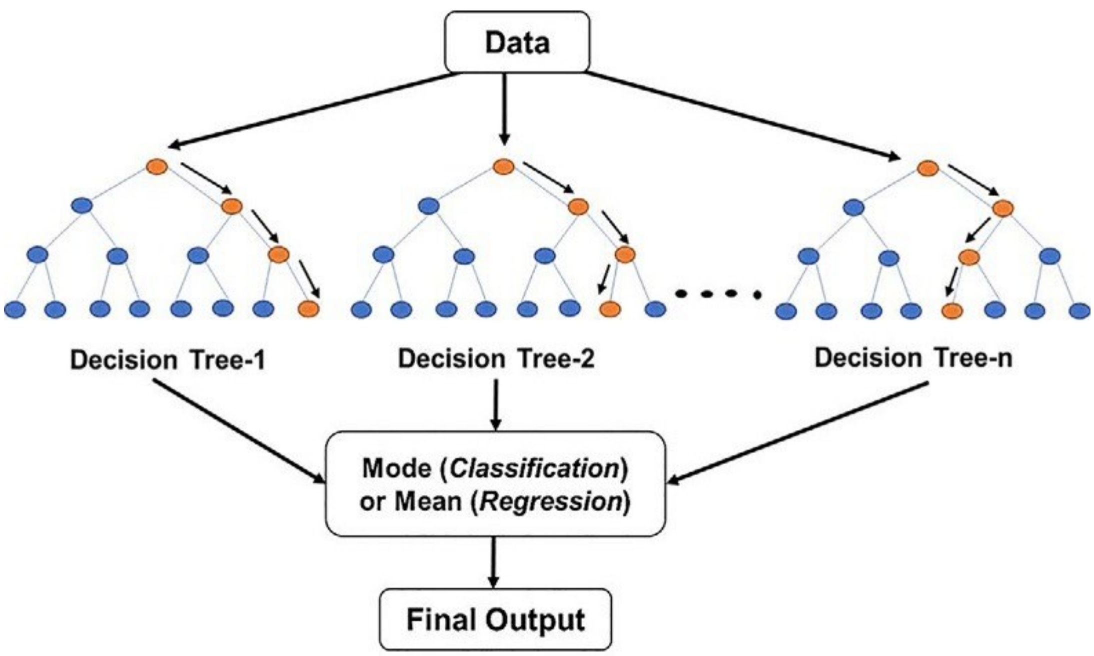

Figure 7. Random Forest model [33]

Apart from prediction, ML models can be combined with optimization algorithms, like Genetic Algorithms (GA) and Particle Swarm Optimization (PSO). The hybridization of ML with optimization algorithms allows us to find optimized parameters that lead to

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increased fluxes and reduced fouling or power costs. In other words, by applying ML models along with optimization algorithms, we do not require experiments anymore.

3.4 Bayesian Neural Networks and Uncertainty Quantification

While conventional ANN models provide deterministic predictions, Bayesian Neural Networks (BNNs) extend this capability by incorporating probability distributions into model parameters, enabling uncertainty quantification alongside performance prediction. This feature is particularly valuable in MD applications because industrial wastewater characteristics often vary with production activities, feed composition, and operating conditions. Unlike conventional models that generate a single prediction value, BNNs provide prediction confidence intervals that indicate the reliability of model outputs [21].

The ability to quantify uncertainty supports risk-based decision making in MD systems. For example, operators can evaluate the likelihood of flux decline, membrane wetting, or performance deterioration before implementing operational changes. Such probabilistic information improves process reliability and assists in developing more robust control strategies for treating highly variable industrial wastewater streams, including pulp and paper effluents [20].

3.5 Monte Carlo Simulation for MD Risk Assessment

Monte Carlo simulation is a statistical technique widely used to evaluate uncertainty and risk in complex systems. In MD applications, the method repeatedly samples input variables from predefined probability distributions to assess the influence of fluctuations in operating conditions, membrane properties, and feed characteristics on system [21].

Monte Carlo analysis can be used to evaluate uncertainties related to feed temperature variation, membrane degradation, and fouling development, all of which may affect permeate flux and rejection efficiency. Furthermore, Monte Carlo simulation can be integrated with ANN and BNN models to improve prediction reliability by quantifying the probability of different operational outcomes. This hybrid approach enables better risk assessment, supports proactive maintenance planning, and enhances operational decision making under uncertain wastewater treatment conditions [18, 20].

3.6 Evaluation Metrics for ML Models

To evaluate the efficiency and validity of ML algorithms applied in MD systems and wastewater treatment processes, several statistical performance metrics are commonly employed. These metrics assess the accuracy, robustness, and predictive capability of models used to estimate key process indicators, such as permeate flux, rejection efficiency, fouling tendency, and membrane performance under varying operating conditions. The coefficient of determination (R^2), which is frequently employed, is the statistic used for quantifying the ratio of variance of data described by the model to the total variance in the data. A greater value of R^2 implies a better accuracy of the algorithm.

Moreover, there are some error measures such as Root Mean Square Error (RMSE) and Mean Absolute Error (MAE). RMSE is very sensitive to extreme prediction differences since it squares all errors, whereas MAE simply evaluates the absolute error size. Both

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criteria provide an adequate assessment of the accuracy of the predictions performed by the model [34]. Model accuracy and reliability are evaluated using statistical indicators, namely mean squared error (MSE), mean absolute error (MAE), root mean squared error (RMSE), mean absolute percentage error (MAPE), and the coefficient of determination (R^2), defined as:

$$MSE = \frac{1}{n}\sum_{i=1}^{n}(y_i - \hat{y}i)^2 \tag{1}$$

$$MAE = \frac{1}{n}\sum i = 1^n |y_i - \hat{y}i| \tag{2}$$

$$RMSE = \sqrt{\frac{1}{n}\sum i = 1^n (y_i - \hat{y}i)^2} \tag{3}$$

$$MAPE = \frac{100}{n}\sum i = 1^n \left|\frac{y_i - \hat{y}i}{y_i}\right| \tag{4}$$

$$R^2 = 1 - \frac{\sum i=1^n (y_i - \hat{y}i)^2}{\sum i=1^n (y_i - \bar{y}i)^2} \tag{5}$$

where mean of experimental values, and *n* is the number where *yi* are experimental values, $\hat{y}_i$ are predicted values, $\bar{y}$ is the of data points.

3.7 Summary of Machine Learning Applications in MD

Table 5 gives an overview of important ML techniques used in MD systems and their performance, benefits, and drawbacks. ANN models achieve great results in terms of prediction but lack interpretability, hence known as the "black box problem." SVM models perform better when small amounts of data are available but could be generalized weakly, whereas ensemble learning techniques like RF improve robustness but need a large amount of data. Bayesian techniques like BNN take the latter step further by adding uncertainties, though they become more computationally expensive [35]. Figure 4 until 7 are the representations of ML models that provide insight into how different algorithms capture nonlinear relationships between operating conditions and MD performance. These visual tools support the understanding of model structure, feature interactions, and prediction mechanisms, which are essential for interpreting MD system behavior.

Although there have been considerable advances in ML applications in MD, some challenges persist. Most of the existing studies consider desalination or synthetic wastewater treatment scenarios, with only a few works considering more complicated industrial wastewater such as pulp and paper wastewaters. In addition to that, lack of availability of benchmarking data sets and poor generalizability of ML models are other major drawbacks. Lack of proper quantification of uncertainties is another significant issue which remains unresolved yet. Modern methods like Bayesian learning and Monte Carlo simulation are less explored areas of study here. The need for the hour is an integrative framework of modelling which incorporates both physical and ML knowledge.

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Table 5. Summary of Machine Learning Applications in Membrane Distillation

ML Model	Application	Key Findings	Limitations	Ref.
Artificial Neural Network (ANN)	Permeate flux prediction	Achieved high prediction accuracy under varying operating conditions	Limited dataset size	[17]
Artificial Neural Network (ANN)	DCMD modelling	Outperformed traditional empirical models in flux prediction	Black-box issue (limited interpretability)	[16]
Bayesian Neural Network (BNN)	Uncertainty analysis	Provides probabilistic outputs with confidence intervals	High computational cost	[35]
Random Forest (RF)	Fouling prediction	Identifies key variables influencing performance degradation	Requires large dataset	[33]
Support Vector Machine (SVM)	Permeate flux prediction	Effective for small datasets and nonlinear modelling	Limited generalizability	[36]

4.0 MACHINE LEARNING PERFORMANCE PREDICTION AND OPTIMIZATION IN MEMBRANE DISTILLATION

4.1 Permeate Flux Prediction

ML technologies have greatly improved the accuracy of prediction of flux in MD systems due to the capability to apply data-driven modelling techniques to model complicated process characteristics. In contrast with frameworks, where emphasis is placed on structural aspects of the model and its parameters, prediction of flux behaviour by applying ML involves finding the correlation between changing process conditions and flux. MD processes exhibit strong dependence on the feed temperature, feed flow rate, feed salinity, and feed content of organic compounds, especially in cases of wastewater treatment, such as pulp and paper industry effluents.

ML algorithms have been extensively used in predicting the behavior of flux in relation to changing process conditions through the discovery of nonlinear dependencies from data [16,17]. ML algorithms, especially ANNs, can predict the flux decay pattern that emerges due to increasing organic load and concentration polarization and is difficult to model with the help of empirical correlations. In conclusion, modern ML techniques enable the development of dynamic flux prediction models, allowing for accurate predictions of flux change in time as a response to certain process conditions.

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4.2 Rejection Efficiency Modelling

In addition to the use of ML for flux prediction, models are developed to assess the efficiency of rejection by MD systems, especially for those wastewater flows that are more heterogeneous. In theory, MD can achieve almost 100% rejection of non-volatile components; however, depending on the operation of the system and membrane properties, the separation efficiency varies significantly.

ML offers an efficient tool for prediction of rejection efficiency, where the system's input data correlates to the output separation results. Particularly, such modeling becomes relevant for pulp and paper mill effluents with multiple contaminants like lignin, resin acids, dyes, and trace metals. The assessment of multivariate interactions makes it possible to predict rejection performance for varying feed streams and operational conditions [16].

Moreover, the application of the ensemble learning technique such as Random Forest (RF) or Gradient Boosting Machine (GBM) allows us to reveal key predictors contributing to rejection efficiency [33,35]. It is important both from the point of view of increasing accuracy and gaining process knowledge for further optimization of the process. Thus, machine learning based rejection modeling helps to select optimal regimes for MD operations combining high fluxes and high rejection levels.

4.3 Fouling and Wetting Early Warning Systems

Early detection of fouling or membrane wetting events is one of the more interesting applications of ML for the operation of MD systems. These are major problems faced during the process operation that cause flux degradation, deteriorating the efficiency of the membranes as well as potentially compromising their ability to retain separation. Monitoring systems based on ML algorithms use real-time process data to detect the trends of occurrence of fouling or wetting incidents. Variations of such operational parameters as permeate flux, temperature gradients, and permeate conductivity may be analyzed to detect changes occurring at early stages, prior to permanent damage to the performance of the system [13].

Furthermore, the use of probabilistic ML algorithms, like Bayesian networks, improves the capacity to detect such events through incorporating probability within the predictive model. In essence, such models provide not a point forecast, but rather an estimation of the probability of a certain event occurring [35]. It is especially valuable due to compositional variability of wastewater. Implementation of early warning systems using ML techniques in MD operations allows shifting from preventive to proactive maintenance approaches. In addition to process reliability, costs and membrane life can be improved as well, thus rendering ML an indispensable element for future intelligent MD system.

4.4 ANN-Assisted Optimization of PVDF/CNC Composite Membranes

Advanced membrane materials play an important role in mitigating fouling, wetting, and flux decline in MD systems. Among them, PVDF membranes modified with cellulose nanocrystals (CNCs) have gained attention due to their improved porosity, hydrophobicity, mechanical strength, and antifouling properties. These enhancements contribute to better

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MD performance, particularly for treating complex industrial effluents such as pulp and paper wastewater [37,38].

The incorporation of CNC introduces several interacting variables, including membrane porosity, pore size distribution, contact angle, membrane thickness, and operating conditions, making performance prediction challenging using conventional empirical models. ANN provide an effective solution by capturing complex nonlinear relationships directly from experimental data [20,21].

In PVDF/CNC systems, ANN models can predict key performance indicators such as permeate flux, rejection efficiency, thermal efficiency, and fouling tendency based on membrane properties and operating parameters. For example, moderate CNC loading may enhance porosity and vapor transport, whereas excessive loading may reduce hydrophobicity or create structural defects. ANN models can identify these trade-offs and determine optimal membrane formulations with improved performance and fouling resistance [18,20].

Furthermore, ANN-assisted optimization can reduce experimental effort by rapidly predicting membrane performance under different conditions, accelerating membrane development and process optimization. This integration of ANN modelling with PVDF/CNC membrane design offers a promising pathway toward intelligent and reliable MD systems for pulp and paper wastewater treatment [18,21].

5.0 CURRENT TRENDS, CHALLENGES AND FUTURE PERSPECTIVES

5.1 The "Black Box" Problem and the Need for Explainable AI

Although ML models have very good prediction power in the case of MD process, one of the most serious disadvantages is the inability of ML models to provide any physical insights about the process. This problem is termed the "black box" problem in the literature. In other words, many machine learning methods, especially ANNs and Deep Learning Algorithms, can be very effective in predicting the output variables but do not provide any information about the physical interactions of the process [16,17].

To solve this problem, much attention has recently been paid to the development of XAI (Explainable Artificial Intelligence) techniques, which are used to deliver interpretable results of prediction algorithms. The use of XAI provides opportunities to analyze key input factors affecting the model, thus making it more user-friendly for engineers. Moreover, new solutions like PINNs (Physics-Informed Neural Networks) combine the principles of data-driven models and physical laws that make ML predictions thermodynamically and kinetically feasible [39]. This type of modelling is especially relevant to MD since it allows combining heat and mass transfer processes and data-driven learning, leading to enhanced prediction capabilities and greater interpretability of results.

5.2 Data Scarcity and Generalizability Challenges

Another important limitation that restricts the wide use of machine learning in MD systems is insufficient large-scale and high-quality datasets. Most of the machine learning studies utilize small sample size datasets or artificial datasets created within the lab experiments. These datasets have significant value for model training, but unfortunately,

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they cannot fully reflect the complex nature of industrial wastewater, especially pulp and paper wastewater [16,35].

The real process of pulp and paper wastewater treatment involves significant variations in the content of contaminants, operating temperatures, and other factors, which influence the efficiency of MD treatment systems. But at the same time, long-term datasets that can fully cover this variability are rare. It leads to problems with model generalization because the dataset-specific algorithms can work adequately only in the similar settings. For overcoming this problem, future research should pay special attention to developing standardized high-quality datasets based on industrial and pilot-scale tests. Moreover, hybrid modelling that combines ML models with physical models will be helpful for ensuring the generalization since this approach incorporates physical limitations into machine learning.

5.3 Digital Twins and Smart MD Systems

One of the most promising trends in the application of ML in MD systems is the development of digital twins virtual replicas of physical processes that enable real-time monitoring, prediction, and optimization. Digital twins make use of ML models in tandem with real-time data obtained from sensors to simulate various working scenarios of a given system under different operational conditions.

With regards to the issue of wastewater treatment in pulp and paper industry, ML-powered digital twins may be employed for continuous monitoring of important performance metrics including permeate flux, rejection efficiency, and fouling behavior. As a result of simulations provided by predictive models, an operator will have the opportunity to adjust process parameters in advance, thereby avoiding any possible problems with the process and switching from reactive to predictive control [33,35].

Furthermore, the integration of digital twins with advanced control systems enables automated optimization of MD processes, reducing operational costs and minimizing human intervention. As sensor technologies and data acquisition systems continue to improve, the implementation of digital twin frameworks is expected to become more feasible for large-scale industrial applications. Ultimately, the adoption of ML driven digital twins represents a significant step toward the development of intelligent and autonomous wastewater treatment systems for the pulp and paper industry.

To conclude, while machine learning techniques have proven themselves highly effective when it comes to the prediction and optimization of MDs, there is still much work to be done. Some of the major problems associated with machine learning in this context include explainability, data access, and scalability. Fortunately, developments in the field of explainable AI, physics-informed modeling, and digital twins may prove useful in addressing these issues.

6.0 CONCLUSION

Recent developments in ML techniques have greatly impacted the use of MD for wastewater treatment by shifting the technique from a reactive to a predictive mode. It has been shown that ML models possess significant predictive power in relation to important MD parameters such as permeate flux, rejection efficiency, and fouling characteristics,

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even under highly fluctuating conditions as is common for wastewater produced in the pulp and paper industry. Through its capability of describing complex, non-linear relations, ML minimizes the need for costly experiments and facilitates the development of efficient processes.

ML technologies have increased the possibility of detecting performance losses and system instability in a timely manner by means of predictive modeling and warning systems. Furthermore, the inclusion of probabilistic techniques such as Bayesian methods allows for the modeling of uncertainties, thus facilitating decision making. ML optimization procedures have been shown to allow for determining optimum operational conditions with respect to achieving a good balance between high permeate flux and high rejection efficiency while minimizing energy consumption.

Notwithstanding the potential, there are certain challenges that need to be overcome prior to the full-scale application of ML-enabled MD systems in the pulp and paper industry. The main problems in this area involve insufficient availability of industrial data on a large scale, poor generalization capabilities of ML algorithms, and the lack of interpretability of complex models often described as black boxes. The solution to all the difficulties will necessarily lie in the development of more explainable and physics-enabled modeling techniques. The synergy of ML and real-time monitoring, as well as the use of digital twin technology, will become crucial for taking MD to the next stage of its evolution practical implementation in the industry. Digital twins based on ML can help track system performance and carry out maintenance and optimization processes, thus leading to higher reliability and lower operational costs. In summary, although MD is a well-grounded technology that can be used to treat complicated industrial wastewater, its maximum potential will only be achieved by incorporating ML into it.

DECLARATION OF COMPETING INTEREST

The authors declare that the work reported in this study was not affected by any conflicting financial interests or personal connection.

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