



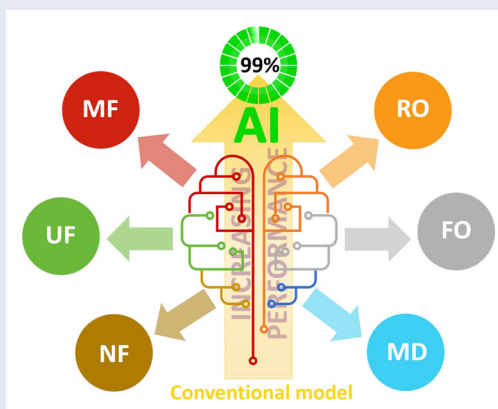
Enhancement of membrane system performance using artificial intelligence technologies for sustainable water and wastewater treatment: A critical review

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ABSTRACT


In recent years, membrane technologies are widely utilized in water and wastewater treatment processes. However, controlling and improving these systems still need to be investigated and, therefore, are attracting increasing amounts of attention from researchers worldwide. Industry 4.0 has increased in importance over the past few years, and artificial intelligence (AI) technology has demonstrated its strength in supporting decision-making in various fields, including environmental systems and especially membrane processes. AI allows for cost-effective operation of systems, including better planning and tracking as well as comprehensive understanding of resource-loss in real-time, then maximizing revenue capture and water quality satisfaction. This study therefore aims to provide a comprehensive review of the current application of AI-based tools in simulating membrane processes as well as the feasibility of applying these models to other fields in which membranes are to be used in the future. The existing conventional mathematical models are illustrated along with their advantages and shortcomings. The definition and classification of state-of-the-art AI models, as well as the benefits of these over conventional models, are also discussed. Furthermore, the basic principle of membrane processes and current application of AI-based technologies in simulating the performance of these membrane systems are systematically reviewed. Finally, the implications and recommendations for future studies are discussed.



KEYWORDS Artificial intelligence; Industry 4.0; membrane processes; modeling; sustainable water treatment

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1. Introduction

Climate change has altered the scenario regarding water resources over recent decades, rendering water scarcity a global challenge. The demand for water is predicted to grow at a rate of 1% per year in all sectors (S. Im et al., 2020; UN-Water, 2018). The reuse of water and wastewater therefore plays a pivotal role in satisfying the global water demand for sustainable development in the context of a circular economy.

The United Nations has proposed actions to achieve clean water and sanitation for all by 2030 in Goal 6 of its Sustainable Development Goals, which includes the effective reuse of water and wastewater. Reusing wastewater and seawater desalination are the major sustainable water resource production methods that have the capability to meet the continuously increasing demand for fresh water. Membrane-based technologies have emerged as viable solutions that can deal with water shortages and security (Yusuf et al., 2020). To optimize and design an economical and effective system, the current membrane processes are normally integrated with an automatic system that can regularly adjust parameters during operation (i.e., flow rate, pressure, pH, cleaning methods and procedures, etc.), which is performed online and is a real-time process. However, the current systems do not satisfy the requirements for increasing accuracy and improving timelines (due to the data collected cannot provide a predictive information of the system performance and the system cannot analyze data to send a signals for operators in time); consequently, the creation of models that can accurately predict the performance of a system has become necessary. Conventional models usually utilize mathematical or empirical methods as estimation techniques for control systems. Although these models may result in practical functions that can be used in the rapid optimization of a process (Luis & Van der Bruggen, 2015), they still have several limitations owing to the complexity and nonlinearity of the architecture (Asghari et al., 2020). For example, conventional models are normally based on several assumptions, which may lead to low accuracy in predictions compared to those that use a real dataset (Q. Liu & Kim, 2008). In addition, mathematical models may include misunderstandings of general dynamic phenomena, resulting in a low fit between predicted and actual data. Empirical models are also generally based on specific experimental data that are collected from local systems. The predicted results may therefore differ significantly for other systems because of the differences in operating conditions, the chemicals utilized, and the equipment used in a plant (Lipnizki & Tragardh, 2001). Meantime, artificial intelligence (AI) technique has recently emerged as an alternative method for simulation of the performance of membrane processes.

The innovation surrounding Industry 4.0 means that AI strategies are very high on the agenda of many developed governments (Ahmad et al., 2021), with developing AI technologies playing a vital role in scientific research, the private and public sectors, education, infrastructure, and the environment. AI-based model strategies could therefore be an alternative method for simulating membrane systems (Soroush et al., 2018). Such models can detect objects in images, conduct facial recognition, carry out natural language processes, improve robotic systems, and even diagnose disease (Guo et al., 2019). AI normally uses a set of algorithms to solve problems, which is totally and automatically performed by a computer, while conventional models are built in a time-consuming process by solving a series of functions by hand. In comparison to conventional mathematical models, AI models are able to tackle complex nonlinear regression issues and produce an accurate mechanism of the overall dynamics involved in membrane processes. In addition, AI techniques are a timely and acceptable cost method for predicting system performance (i.e., by reduction of complicated analysis of several operating parameters). These modern techniques also play an indispensable role in optimizing the parameters that are involved in the process by performing independent data processing, providing output based on the input dataset, adjusting the action of a series of equipment, and providing information for the production of timely and automatic decisions (Bunmahotama et al., 2017), then reducing the additional cost for maintenance as well as fixing the system in the case that unexpected events occurred suddenly. Environmental systems, particularly membrane process performance, can be simulated using AI tools.

The number of publications examining the application of AI-based techniques in membrane processes for water and wastewater treatment has rapidly increased over recent years, with the number of papers produced in the year 2020 is 7 times higher than that in 2016 (Figure 1). However, reviews describing the utilization of AI techniques to investigate the performance of membrane processes for water and wastewater treatment are rare in the literature. Previous studies have only reported the application of artificial neural network (ANN) techniques in the drinking water sector or gas separation processes (Li et al., 2021; O'Reilly et al., 2018). Moreover, the benefits of using AI models in comparison to conventional mathematical models and their application in all membrane processes have not been investigated. This article therefore aims to provide a systematic review of the application of AI-based techniques in simulation of the membrane processes for water and wastewater treatment for the first time. Conventional mathematical models that are used for membrane separation processes, as well as their advantages and disadvantages, are briefly

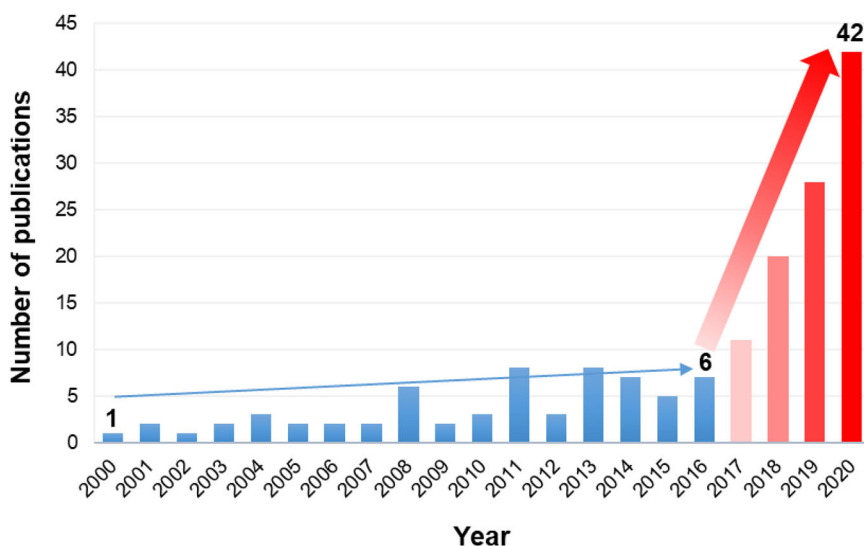


Figure 1. Publications reporting AI application in membrane processes (Data source: Web of Science).

described. The definition and classification of state-of-the-art AI-based techniques as well as the benefits and drawbacks of these techniques in comparison to conventional models, are also emphasized. Finally, the principles of membrane-based technologies and application of AI-based models to examine the performance of these membrane processes in water and wastewater treatment are critically discussed with current trends and future prospects are provided.

2. Existing mathematical models for predicting the performance of a membrane process

2.1. Representative models

Mathematical models that are used to simulate MF currently focus on fluxes and permeabilities rather than contaminant removal efficiency (Van der Bruggen, 2018). The process used to model water flux (dead-end mode) through a cylinder can be represented by the theoretical Hagen-Poiseuille model, while the flux in non-cylindrical models can be defined using the Ergun equation. Water permeance depends on the transmembrane pressure, membrane resistance, and fouling resistance, as shown in Eq. (1) (Table 1). The final equation describing water flux in the crossflow mode of the MF process is given in Eq. (2) (Table 1). The mathematical models of MF that are used in water and wastewater treatment have been widely applied in several studies (Davis, 1992; Polyakov & Zydney, 2013; Rahimi et al., 2005).

Table 1. Existing mathematical models for membrane processes

| Equations | 1. MF (Davis, 1992; Van der Bruggen, 2018) | Equations | 2. UF (Mochizuki & Zydney, 1992; Van der Bruggen, 2018) | Equations | 3. NF (Van der Bruggen, 2018) |
|------------------------------|--|--------------------------------|---|-----------------------------------|--|
| (1) Flux with dead-end mode | $N = \frac{1}{\eta} \cdot \frac{\Delta P}{R_m + R_c \delta_c + R_f}$ | (3) Water flux | $N = \frac{\pi \Delta P}{8 \eta l_p} \int_{r_p^{min}}^{r_p^{max}} n(0) f_n(r_p, 0) \exp\left(-\frac{\pi \Delta P}{8 \eta l_p} r_p^4\right) \int_{r_p}^{r_p^{max}} c(r_s) dr_s r_p^4 dr_p$ | (5) Water flux | $N = -A \cdot \left(\frac{dp}{dx} - \sum c(1 - \tau_i) \frac{d\mu_i^{(e)}}{dx} \right)$ |
| (2) Flux with crossflow mode | $N = \frac{\Delta P}{\left(\frac{\Delta P \Phi_b \eta R_c}{k_1 \left(\frac{\Phi_c}{\Phi_b} \right)^2} \left(1 - \exp\left(-\frac{2k_1 \left(\frac{\Phi_c}{\Phi_b} \right)^2}{\Phi_c - \Phi_b} \right) \right) \right)^{0.5} + \eta \cdot (R_m + R_f)}$ | (4) Final conc. of contaminant | $c(r_s, t) = c(r_s) \frac{\int_{r_p^{min}}^{r_p^{max}} S_i \frac{d\mu_i^{(e)}(t)}{f_n(r_p, t)} r_p^4 dr_p}{\int_{r_p^{min}}^{r_p^{max}} n(t) f_n(r_p, t) r_p^4 dr_p}$ | (6) Flux of a dissolved component | $N_s = -\frac{B}{RT} c \left(\frac{d\mu_i^{(c)}}{dx} - Z_i \sum_l \frac{t_l}{Z_l} \frac{d\mu_l^{(c)}}{dx} \right) + NT_i c$ |
| Equations | RO (J. Wang et al., 2014) | Equations | FO (Manickam & McCutcheon, 2017) | Equations | MD (DCMD) (Perfilov, 2019; Qi et al., 2020; Schofield et al., 1990) |
| (7) Water flux | $N = A(\Delta P - \Delta \pi)$ | (9) Water flux | $N = A \left[\frac{\pi_D \exp\left(-\frac{N}{k_f}\right) - \pi_d \exp(NK)}{1 + \frac{B}{N} \left[\exp(NK) - \exp\left(-\frac{N}{k_f}\right) \right]} - \Delta P \right]$ | (11) Vapor flux by mass transfer | $N = \left(\frac{1}{(a_{Sch}(P_M/P_{ref}))^{b_{Sch}}} + \frac{P_d}{\tau_i} \right)^{-1} \Delta P$ |
| (8) The solute flux | $N_s = \frac{\tau_i K C_d}{\Delta x} \left(1 - \exp\left(-\frac{v_i [\Delta P - \Delta \pi]}{RT}\right) \right)$ | (10) The salt flux | $N_s = B \left[\frac{\pi_D \exp\left(-\frac{N}{k_f}\right) - \pi_d \exp(NK)}{1 + \frac{B}{N} \left[\exp(NK) - \exp\left(-\frac{N}{k_f}\right) \right]} \right]$ | (12) Vapor flux by heat transfer | $N = \frac{h_v}{\Delta H_v} \frac{h}{h_v + h_c + h} (T_f - T_p)$ |

N (water flux); N_s (solute flux); ΔP (transmembrane pressure); $\Delta \pi$ (osmotic pressure); π_D (DS osmotic pressure); η (feed viscosity); A (solvent permeability); B (ion permeability); R_m , R_c , R_f (membrane, cake layer, and fouling resistances); δ_c (cake layer thickness); Φ_b , Φ_c (suspension and cake solid volume fraction); k_1 (fitting parameter); $\frac{d\mu}{dy}$ (velocity gradient); l_p (membrane thickness); r_p^{max} , r_p^{min} (maximum and minimum pore radius); $n(t)$ (total number of the open pore/m² at t); $f_n(r_p, t)$ (probability density function); $c(r_s)$ (contaminant density); S_i (sieving coefficient); k_f (mass transfer coefficient); c (salt conc. in the permeate); $\mu_i^{(e)}$ (ion electrochemical potential); x (membrane coordinate); τ_i (ion diffusion coefficient); T_i (ion diffusion coefficient at zero electric current); v_i (number of ions in dissociated salt); Z_i (ion valance); K (liquid-phase sorption coefficient); a_{Sch} (permeation constant); P_M , P_{ref} , P_d (average pressure of membrane pores, reference pressure, air within membrane); b_{Sch} (exponent defines Knudsen diffusion); h , h_c , h_v (film, vapor, conductive heat transfer coefficient); ΔH_v (latent heat of vaporization); T_f , T_p (feed & permeate temperature).

Unlike MF, the conventional models describing UF have focused on the rejection of contaminants, referring to the MWCO of a membrane. Polyakov and Zydney (2013) developed a hydrodynamic equation for the movement of a single salt ion in a pore (Polyakov & Zydney, 2013). The final flux equation for this process is given in Eq. (3) (Table 1), and it is dependent on the membrane thickness, pore radius, and the viscosity of the feed stream. The final concentration of a contaminant can also be calculated using Eq. (4). UF models have been utilized to simulate system performance in several recent studies (Mochizuki & Zydney, 1992; Monfared et al., 2012).

The modeling process for NF is complicated due to the steric effect, which combines with charge interactions on a molecular scale. The major principle used in the transport and removal of ions is irreversible thermodynamics, as presented by Yaroshchuk et al. (2019). The final equations describing the fluxes of both water and dissolved components that have been developed in this model are given in Eqs. (5) and (6), respectively, as shown in Table 1. These equations have been used in studies modeling NF for desalination and wastewater treatment (R. Wang et al., 2012; Yaroshchuk et al., 2019).

The theory of solution diffusion, which was introduced by Wijmans and Baker (1995), is generally used to describe the RO process. Equations (7) and (8) in Table 1 generate the final water flux and solute flux, respectively. The transportation of water and salt ions during RO depends on the hydraulic permeability of the membrane, TMP, osmotic pressure, properties of the ions present, and the concentration. The application of the method that is used to simulate RO can be found in the literature (Tong et al., 2020; J. Wang et al., 2014; Wijmans & Baker, 1995).

FO uses a similar principle to that of RO, with the only difference in the transport of water, which occurs via natural “osmotic” pressure. The same transport model as that used for RO could be used for FO modeling, but different parameters would be required. Manickam and McCutcheon (2017) reported the influence that these phenomena have on the FO process to produce the final mathematical models that are presented in Eqs. (9) and (10), respectively (Table 1), which have been utilized to model FO in the literature (Kahrizi et al., 2020; Manickam & McCutcheon, 2017).

In MD, mass transport is carried out by a combination of convection (or advection) and diffusion and, in some cases, phase changes that occur between compartments (Perfilov, 2019). One of the most well-known mathematical models in DCMD is Schofield’s model, which was first proposed in 1987 (Schofield et al., 1987), with further improvements made in 1990 (Schofield et al., 1990). The authors conducted a series of experiments and derived a semi-empirical equation to illustrate the transmembrane vapor

flux, as seen in Eq. (11), [Table 1](#). In addition to the mass transfer theory, the final equation for vapor flux by heat transfer can be expressed using Eq. (12). This method has been used by several authors to simulate MD in previous studies (J. Liu et al., [2021](#); Qi et al., [2020](#); Schofield et al., [1987, 1990](#)).

2.2. Advantages and shortcomings

Mathematical modeling plays a vital role in predicting the performance of membrane processes. The use of mathematical modeling in the simulation of real processes and situations has provided us with several benefits, including process control and design, system optimization, predictions used to plan experiments, and the determination of parameters that cannot be measured directly. The advantage of these models is that basic variables that can be directly observed from experiment are included. In addition, mathematical models result in a structural comprehension of the processes and variables involved (Asghari et al., [2020](#)).

Apart from the benefits, there are several drawbacks to using mathematical models that require consideration. For example, most of the models developed so far have used data from one experiment only under specific operational conditions, which may result in errors when the model is applied in other research (i.e., the model is too specific). In addition, the too many variables are generally included in mathematical models, resulting in a complicated series of equations. The development of conventional models is complex and many steps are generally required to achieve the final equations, rendering the modeling process time-consuming. The conventional models used to simulate membrane processes are also highly dependent on the specific mechanism of the process as well as the principle of separation. For example, the complicated relationship between heat and mass transfer in MD results in a low prediction accuracy (Hitsov et al., [2015](#)).

To solve the drawbacks of conventional mathematical models, novel artificial intelligence-based technology has been proposed as a strong and effective tool that can be used to simulate membrane processes for use with desalination and wastewater treatment in the future.

3. State-of-the-art Artificial intelligence-based models

3.1. Definition and classification

AI can be defined as the intelligence represented by a system that imitates the natural intelligence of humans (Altinkaya et al., [2014](#)). AI-based models have been widely used for the simulation and optimization of complicated

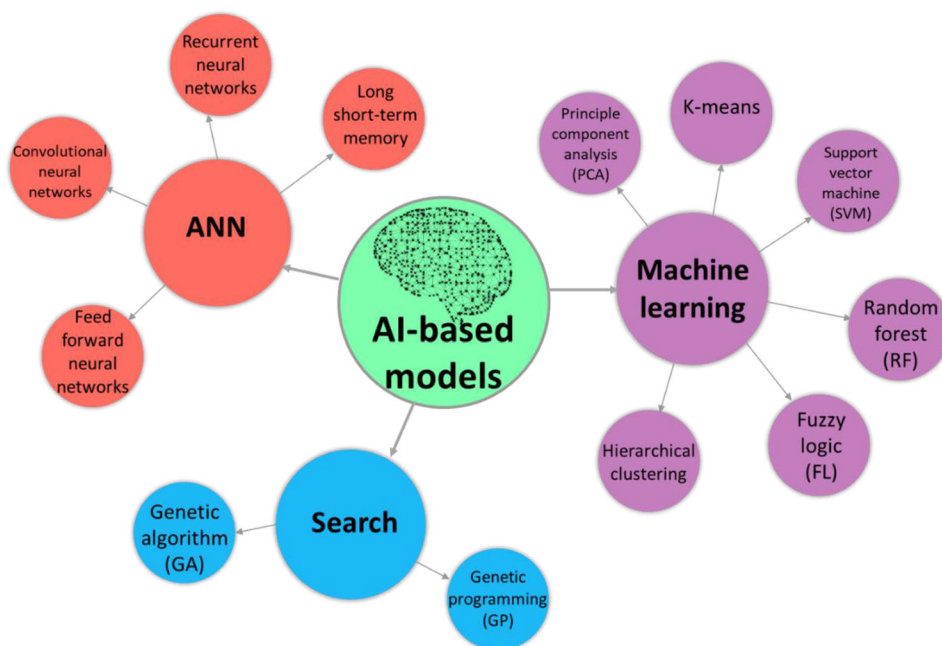


Figure 2. The classification of AI-based models that are applied in membrane systems for water and wastewater treatment.

issues in various areas of science and technology, such as controlling energy systems (Timur et al., 2020), health (Siuly & Zhang, 2020), agriculture (Eli-Chukwu, 2019), and the corona virus (COVID-19) pandemic (Jakhar & Kaur, 2020). AI-based models have also been applied in several environmental systems, including membrane processes. The methods are based on non-parametric algorithms that imitate natural functions of the human brain, such as learning and problem solving.

Generally, the AI-based models that are used to predict the performance of membrane processes can be classified into three groups: machine learning (ML), ANN, and search algorithms (see Figure 2). Machine learning utilizes algorithms that analyze data, then learn from it and use the knowledge from learning process to summarize trends or patterns of interest, while an ANN is more complexed, it comprises a set of algorithms that used in ML for data modeling using a network of hidden layers and neurons. ML is commonly utilized to solve problems involving regression, classification, clustering, or dimensionality reduction (Li et al., 2021). Principal component analysis (PCA) is a dimensional reduction method used in ML that is normally utilized to solve high-dimensional datasets (Antonopoulos et al., 2020). The K-means algorithm is a distance-based method that is commonly used in clustering items to predict which points are at the center of a cluster and label each data point in the set (Zhou et al., 2016). Another ML method is the support vector machine (SVM), which strongly

supports mathematical theory. SVM is able to deal with optimization problems, ensuring the overall capability of an algorithm and avoiding the problem (Chen et al., 2013). Random forest (RF) is commonly used to perform nonlinear classification and regression analysis; it is also able to evaluate the importance of a variable while conducting a classification or regression analysis. Fuzzy logic (FL) is a multivalued logic ML method that is used for studying fuzzy judgment. The combination of FL and ANN, referred to as ANFIS, is commonly utilized in predicting system performance. Hierarchical clustering is a cluster analysis technique that classifies to construct a group of clusters and is normally used in segmentation problems (Ikeda & Nishi, 2016; Kwac et al., 2014). So far, several methods in ML such as RF, FL, SVM, or ANFIS have been effectively utilized in simulation of membrane processes (i.e., NF, RO, FO). The detail information will be deeply discussed in Sec. 4.

Four main types of ANN models are available: feed-forward neural networks (FF-ANNs), convolutional neural networks (CNNs), recurrent neural networks (RNNs), and long short-term memory (LSTM). ANNs are computational models that are inspired by biological neural systems. The connections between the units create a directed acyclic graph in FF-ANNs, while RNNs allow for feedback connections, creating a directed cyclic graph (Antonopoulos et al., 2020). FF-ANNs and RNNs have been used in predicting system performance, classification, clustering, and facial recognition, among others (Abiodun et al., 2018). Other types of ANN models include long short-term memory (LSTM), which is a type of RNN that can solve better long-term issues, while convolutional neural networks (CNNs) are suitable for processing data with grid-like topology. These models have mostly been applied in regression (Mohi et al., 2015; Y. Wang et al., 2019). Currently, ANN is one of the most popular method which has been employed in prediction the performance of all membrane processes. The earliest application of ANN in membrane simulations makes it becomes the most mature prediction method. The detail will be discussed more in Sec. 4.

The search algorithm includes a genetic algorithm (GA) and genetic programming (GP), which is used for producing the optimal strategy to solve complicated problems under certain theory (Li et al., 2021). These models have been applied to optimize and simulate the biological processes that occur in nature. The major property distinguishes these is the depiction of a program or algorithm. A fixed-length string solution is normally performed by a GA, whereas a tree structure with nested data is generally created using GP. Search algorithms are utilized in various fields of science and technology, such as solving optimization problems in water treatment systems or finding the best ratio of utilizing chemicals (Monroe et al.,

2019; Suh et al., 2011). To date, search algorithm has just been employed in simulation of MF and UF membrane processes due to its' specific function as indicated above. The application will be once again discussed more with further details in Sec. 4.

3.2. Benefits of AI models over conventional models

The major benefit of AI-based models is that they can implicitly solve complicated nonlinear relationships occurring between input and output parameters, allowing the construction of real-time monitoring systems that can monitor, analyze, and predict water quality, and illustrate the process of contaminant transformation, facilitating the identification of future risks.

Models that are based on the AI technique can also calculate water quality parameters that normally require a long time and complicated measuring processes in the laboratory. In addition, AI-based models can be processed without any assumptions about data distribution or the interaction between factors, which are normally required in conventional mathematical models (Olden & Jackson, 2002; Park et al., 2019).

Autonomous learning and self-diagnosis means that AI models are suitable for establishing an excellent feedback and a highly accurate automatic control, which can run an independent analysis, judgment, and predictions according to the input dataset, then perform the actions of a group of equipment or send out relevant warnings that can be used for decision-making in a timely manner (Bunmahotama et al., 2017).

By adapting to rapid changes that occur in the technologies used for water and wastewater treatment, the developed AI models can be updated with fresh datasets, rendering them feasible for use in a constantly changing environment.

AI allows for the strategic and cost-effective operation of systems, including better planning and tracking as well as comprehensive understanding of resource-loss in real-time, then maximizing revenue capture and water quality satisfaction.

However, models that are based on AI technology are still prone to limitations that need to be considered if the performance of a model is to be increased in the future. For instance, AI models fail to explain the interconnectional relationships between physical parameters, which may limit the ability of a model to fit the changes that have been made in building components or systems (Z. Wang & Srinivasan, 2017). Moreover, the development of AI-based models normally requires a large dataset in order to adequately train and test a model with acceptable accuracy. The development process also needs to be conducted by highly qualified scientists who

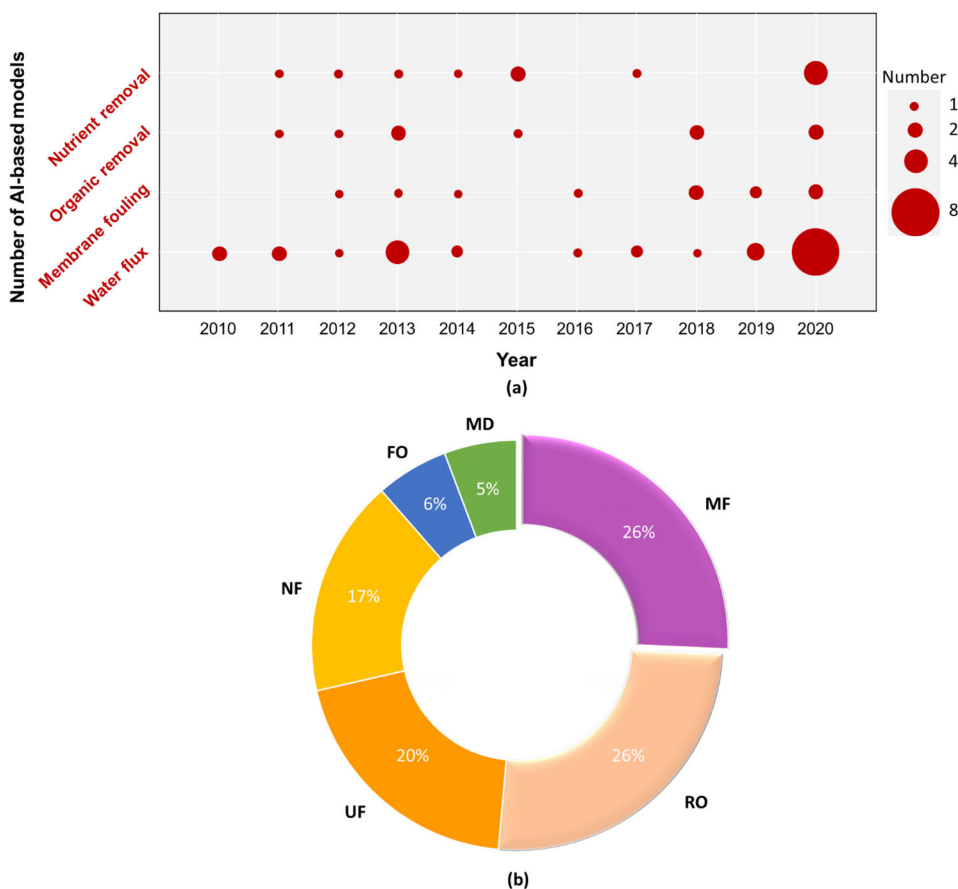


Figure 3. (a) Proportions of AI-based models used in the prediction of membrane filtration performance. (b) Application of AI tools with various types of membrane.

have sufficient knowledge, not only in the environmental aspects, but also in data science technology.

Beyond these limitations, the strengths of AI-based models are still attracting increasing amounts of attention by researchers around the world and the tool has been widely applied in recent years, details of which will be discussed in the following sections.

4. Application of AI-based models in predicting the performance of a membrane system

Currently, models that are based on AI technology are applied widely in the prediction of several performance parameters, including water flux, membrane fouling, and the removal of organic matter and nutrients, as shown in Figure 3(a). Investigation into water flux was particularly intense during the period 2010 to 2020. This may be because water flux is the major and final purpose of all membrane filtration systems. In contrast,

membrane fouling is likely to attract the lowest attention in predictions using AI-based models. This is easy to understand because membrane fouling is an extremely complicated issue that is highly dependent on various operating parameters, leading to difficulties in terms of simulation and prediction. Modeling membrane fouling remains a challenge for researchers. The removal efficiencies of organic matter and nutrients (i.e., nitrogen and phosphorus) appears to have undergone equal investigation over the last decade, producing an average of at least one report per year and contributing to the global knowledge on the potential of applying AI models in simulating the performance of membrane filtration systems.

In order to gain more insight into the potential of AI modeling in the simulation of membrane processes, this study categorizes the application of AI models in accordance with membrane type. As indicated in [Figure 3\(b\)](#), MF and RO account for the largest portion of AI applications in membrane systems with over 26%, while UF and NF are used less, at approximately 20%. The applications of AI in FO and MD are lowest, at approximately 6%.

The application of AI models in each type of membrane process (i.e., pressure-driven membranes, osmotic pressure-driven membranes, and thermal-driven membranes) will be presented in the following sections.

4.1. Pressure-driven membrane processes

The difference in the pressure on the feed side and permeate side is utilized as a driving force for transportation of water across the membrane. There are four major types of pressure-driven membrane processes: microfiltration (MF), ultrafiltration (UF), nanofiltration (NF), and reverse osmosis (RO), as shown in [Figure S1, supplementary material](#).

4.1.1. Microfiltration (MF)

MF membranes have the largest pore size and molecular weight cutoff (MWCO), which range from 0.1–10 μm and 100–500 Da, respectively. These properties mean that this type of membrane has the lowest requirements in terms of pressure (1–3 bar) and the highest permeability (500 LMH/bar) compared to the other pressure-driven membrane processes ([Figure S1a, supplementary material](#)). MF is used in various applications involving the treatment of municipal wastewater (Dittrich et al., 1996), oily wastewater (Masoudnia et al., 2015), whey concentration (Ye et al., 2011), and in the pretreatment of seawater for desalination (Wu et al., 2017).

As previously indicated, MF account for the largest application of AI models to pressure-driven membrane processes. Details concerning the application of these models to pressure-driven membrane processes are

presented in Table 2. AI-based models have been applied to water flux and contaminant removal in the MF process. Ghandehari et al. (2013) utilized FF-ANNs and RFB models to simulate the permeate flux when using the MF process to filtrate bovine serum albumin. In this study, influent characteristics, operating parameters and membrane properties were utilized as input dataset. The models showed an R^2 of over 0.99 for all simulations with RMSE values of 7.58 and 0.0058 for water flux and membrane rejection, respectively, indicating that the neural network has potential as an alternative modeling method that can predict system responses with a high level of accuracy. In addition to ANNs, several researchers have also proposed the application of other AI models for predicting the performance of MF systems. For instance, Madaeni and Kurdian (2011) developed a fuzzy logic and GA model for forecasting water flux and rejection, resulting in a fuzzy GA model with very high accuracy in predicting water flux ($R^2 = 0.920$, RMSE = 70.45) and rejection ($R^2 = 0.972$, RMSE = 15.81). This means that in addition to the ANNs, fuzzy and GA models are also capable of predicting flux and rejection under various MF operating conditions (Madaeni & Kurdian, 2011).

4.1.2. Ultrafiltration (UF)

Compared to MF membranes, the pores in UF membranes are of smaller diameter, ranging from 0.001 to 1 μm , which corresponds with the removal of dissolved compounds with a MW of 20–150 Da. The pressure required for filtration is therefore relatively higher than it is in MF (2–5 bar), and the permeability is at 150 LMH/bar (Figure S1b, supplementary material). UF has been widely applied in the treatment of oily wastewater (Salahi et al., 2011), domestic wastewater (Al Aani et al., 2020), magnet fishing (Petricin et al., 2015), and pretreatment of seawater for desalination (Busch et al., 2009).

Most of the predictions in MF have been developed using ANN models (Chew et al., 2017; Delgrange-Vincent et al., 2000; Krippel et al., 2020; Soleimani et al., 2013). Chew et al. (2017) introduced an ANN model for the prediction of specific cake layer resistance. The developed model provides a highly accurate predicted result with an extremely low RMSE of 9.8×10^{-4} , implying that the ANN model could be an easy method for the implementation of UF membranes in industrial-scale water treatment plants. ANN models were also utilized to create models for the estimation of membrane fouling, with an R^2 of over 0.99, a RMSE of 4.2×10^{-5} (Soleimani et al., 2013), and an accuracy of over 90% (Delgrange-Vincent et al., 2000). In addition to single ANN models, a recent study investigated the potential of hybrid AI-based models in predicting UF system performance. For example, Arefi-Oskoui et al. (2017) proposed a hybrid ANN-GA

Table 2. Application of AI-based models in pressure driven membrane processes

| No. | Membrane processes | Type of model | Inputs | Dataset | Data preprocess | Output | Model performance | Ref |
|-----|--------------------|-------------------------|---|------------------------------|---|---|--|----------------------------------|
| 1 | MF | – RBF – ANN | Protein, pH, TMP, CFV, membrane pore size. | – | – | – Flux decline – Membrane rejection | – Permeate flux: $R^2 = 0.99$, RMSE = 7.58; – Rejection: $R^2 = 0.99$, RMSE = 0.0058. | (Ghandehari et al., 2013) |
| 2 | MF | ANN | Pressure, initial conc., stirrer speed, resistance, pH, Temp. | 6×31 matrix | – | Water flux | $R^2 = 0.98$ (training), $R^2 = 0.91$ (testing). | (Ní Mhurchú et al., 2010) |
| 3 | MF | – SVM – ANN | Solid & additive content, temp, humidity, evaporation time, precipitation temp and time. | 150 points | Normalizing (–1; 1) | – Pure water flux – Rejection of BSA | – Pure water flux: errors 2.84% (SVM); 13.72% (ANN); Rejection of BSA: error 2.37% (SVM); 3.55% (ANN). | (Xi et al., 2013) |
| 4 | MF | Fuzzy logic and GA | Pressure, volume, stirring. | 100 points | – | – Flux – Rejection | – Flux: $R^2 = 0.920$, RMSE = 70.45; – Rejection: $R^2 = 0.972$, RMSE = 15.81. | (Madaeni & Kurdian, 2011) |
| 5 | MF (MBR) | Bandelet neural network | MLSS, sludge particle diameter, EPS, SMP concentration, sludge viscosity, RH and Zeta potential | 55 sets of data | Bat algorithm | Membrane flux and γ | Lowest MSE = 0.095% | (B. Zhao et al., 2020) |
| 6 | MF (MBR) | RBF | BOD, COD, $\text{NH}_4\text{-N}$, TP, HRT, MLVSS, TDS, pH. | 30 points | Scaled to the 0–1 | Effluent BOD, COD, $\text{NH}_4\text{-N}$, TP | – BOD ($R^2 = 0.998$, RMSE = 2.98); – COD ($R^2 = 0.998$, RMSE = 11.23); $\text{NH}_4\text{-N}$: ($R^2 = 0.998$, RMSE = 0.14); TP: ($R^2 = 0.995$, RMSE = 0.11); | (Mirbagheri et al., 2015) |
| 7 | MF (MBR) | ANN | Backwash time and service time. | 90 records | Standardization | Permeate flux | $R^2 = 0.995$ | (Aidan et al., 2008) |
| 8 | UF | Hybrid ANN-GA | Concentration of the PVDF, PVP 29 000, NLDH | 24 points | – | – Water flux – BSA flux – Water recovery | $R^2 = 0.98$ for selected topology | (Arefi-Oskoui et al., 2017) |
| 9 | UF | ANN | Feed turbidity, TMP, filtration time. | 52 samples | – | Specific cake resistance | MSE = 9.87×10^{-4} | (Chew et al., 2017) |
| 10 | UF | ANN | Bulk concentration, TMP, concentration factor | 395 points | Normalization to [0, 1] | – Water flux – Filtration duration | RMSE = 0.59; | (Krippel et al., 2020) |
| 11 | UF | ANN | Water quality parameters, backwash conditions. | 1050 samples | – | Fouling resistance | Accuracy: 90% | (Delgrange-Vincent et al., 2000) |
| 12 | UF | ANN | Temperature, TMP, CFV, pH. | 81 points | – | – Permeate flux – Fouling resistance | – Permeate flux: $R^2 > 0.99$, RMSE = 1.89×10^{-4} ; – Fouling resistance: $R^2 > 0.99$, RMSE = 4.20×10^{-5} . | (Soleimani et al., 2013) |
| 13 | UF (MBR) | SVM | Iron, manganese, fulvic acid, and iron hydroxide concentrations. | 11 datasets | Standardized | Membrane fouling (pressure decline) | $R^2 = 0.95$, RMSE = 7.41. | (Aya et al., 2016) |
| 14 | NF | – ANN – SVM – RF | Membrane types (MWCO, materials, morphology); Solvent types (MW, viscosity, density); Operating conditions (process, concentration, T, P) | 38 430 datasets (67 sources) | – Principal component analysis (PCA) – Spearman's rank-order correlation | Permeation and rejection; Decision rules; Relative importance of system descriptors | – ANN: $R^2 = 0.97$, RMSE = 0.57 (Permeance); $R^2 = 0.99$, RMSE = 4.42 (Rejection) – SVM: $R^2 = 0.94$, RMSE = 0.86 (Permeance); $R^2 = 0.96$, RMSE = 8.78 (Rejection) – RF: Accuracy (A) = 0.98, Kappa (K) = 0.95 (Permeance); A = 0.93, K = 0.85 (Rejection); | (Hu et al., 2021) |



| | | | | | | | | |
|----|--------------|----------------|--|-----------------|------------------------------------|---|---|------------------------------|
| 15 | NF | ANN | Concentration of salt and dye in feed, CFV, feed pressure, pH. | 218 datasets | – Evaluation of correlation | Salt rejection rate | $R^2 = 0.995$, RMSE = 0.031. | (Eren et al., 2012) |
| 16 | NF | ANN | Concentration and TMP. | 30 samples | – | Water flux | $R^2 = 0.9918$. | (L. Zhao et al., 2010) |
| 17 | Hybrid NF-RO | – ANN – RSM | Concentration, pH, temperature, and pressure | 30 set of runs | Analysis of variance (ANOVA) | – Flux; Recovery; Rejection; Specific energy consumption | ANN: $R = 0.98$, MSE = 1.55 (NF); $R = 0.99$, MSE = 0.96 (RO); RSM: $R^2 = 0.95$, 0.96, 0.84, 0.92 for flux, recovery, rejection, SEC. | (Srivastava et al., 2021) |
| 18 | Hybrid NF-RO | CNN | Optical coherence tomography (OCT) images | 13 708 images | k-means clustering | – Water flux – Membrane fouling | – Water flux: $R^2 = 0.98$, RMSE = 1.44; – Fouling thickness: $R^2 = 0.88$, RMSE = 4.64; | (Polyakov & Zydney, 2013) |
| 19 | RO | ANN | Filtration time and total solid concentration | 135 points | Normalized in the range of (–1, 1) | Permeate flux | $R^2 = 0.99$, mean absolute percent error = 2.65% | (Rajabzadeh et al., 2012) |
| 20 | RO | ANN | STM time-interval | 4569 points | Operational logs | – Permeate flux – Salt flux | – Permeate flux: accuracy = 0.70, error = 0.81; Salt: accuracy = 0.85, error = 3.89; | (Libotean et al., 2009) |
| 21 | RO | ANN | Temperature, TMP, Time, Material concentration | 285 points | – | Water flux | – Raw membrane: $R = 0.98$, MSE = 1.11; Modified membrane: $R = 0.99$, MSE = 0.78; | (Farahbakhsh et al., 2019) |
| 22 | RO | ANN | SiO ₂ influent concentration, TDS influent, Time | 144 data points | – | – Permeate flow | Permeate flux: $R^2 = 0.99$, RMSE = 2.83 LMH. | (Salgado-Reyna et al., 2015) |
| 23 | RO | ANN | Time, TMP, conductivity, flow rate | 332 points | – | – Permeate flux and conductivity | – Permeate flux: $R^2 = 0.95$, RMSE = 1.59; Conductivity: $R^2 = 0.99$, RMSE = 1.67. | (Madaeni et al., 2015) |
| 24 | RO | RBF | 9 parameters, including model parameters, membrane properties, and operation conditions. | 304 data | Mehdizadeh and Dickson algorithm | – Separation factor; Pure solvent flux; | – Separation factor: ($R = 0.9998$, MSE = 0.00009); Pure solvent flux: ($R = 0.09995$, MSE = 0.00013); | (Iranmanesh et al., 2016) |
| 25 | RO | ANN | Time, salinity, pressure, membrane type. | 372 points | Correlation evaluation | Water permeability | $R^2 = 0.996$. | (Barello et al., 2014) |

model in order to determine the most appropriate input dataset as well as the simulation of water flux in a UF membrane for water treatment (Arefi-Oskoui et al., 2017). The developed model showed an R^2 of 0.98 for water flux prediction, indicating that the UF membrane could be successfully optimized using the hybrid ANN-GA model.

4.1.3. Nanofiltration (NF)

NF membranes are vastly different from both MF and UF. The typical property of an NF membrane is its surface charge, which facilitates the retention of ionic species (i.e., multivalent ions). Typically, the pore size in NF membranes ranges from 0.001 to 0.01 μm , and can retain contaminants with a MW of 2–20 Da. A pressure of 5–15 bar is required for NF to work, producing a permeate flow of 10–20 LMH/bar (Figure S1c, supplementary material). NF is applied in the treatment of leachate (Rautenbach et al., 2000), textiles (Ellouze et al., 2012), paper mill wastewater (Sun et al., 2015), and the pretreatment of seawater before desalination (Abdelkader et al., 2018).

Unlike MF and UF membrane processes, the application of AI models to NF membrane processes have mainly concentrated on salt rejection, rather than water flux or membrane fouling. Hu et al. (2021) compared three different AI-based models for the prediction of salt rejection in organic solvent nanofiltration. The predicted results showed that of the three proposed models, ANNs demonstrated the highest performance with an R^2 of 0.99 and a RMSE of 4.42. Salt rejection was also considered in a study by Eren et al. (2012), in which the salt rejection rate was predicted from a set of operating parameters. The developed models showed an R^2 of 0.995 and a RMSE of 0.03, indicating that the model was much better than that demonstrated in the study by Hu et al. (2021). This might be because the dataset used in the study by Eren et al. (2012) was much smaller than that used in the study by Hu et al. (2021) (218 samples vs. 38 430 samples, respectively). In addition to the utilization of operating parameters as the input set, a vastly different model that uses real-time optical coherence tomography (OCT) images as an input has also been developed (Park et al., 2019). This model is completely different from previously proposed convolutional neural network (CNN) models. The authors utilized 13 708 OCT images as an input for the model to simulate the water flux and real-time membrane fouling occurring in a hybrid NF-RO system. The developed CNN model demonstrated high performance for water flux ($R^2 = 0.98$, RMSE = 1.44 LMH).

4.1.4. Reverse osmosis (RO)

RO membranes are made of dense material without any predefined pores. This material results in slower permeation (5–10 LMH/bar) that is

accompanied by differences in the rejection mechanism. The low permeability also requires the application of high pressure (15–75 bar) (Figure S1d, supplementary material). RO is widely known for its capability to remove up to 99.5% of small particles (Ezugbe & Rathilal, 2020) and has been utilized in desalination and in the treatment and reuse of wastewater.

Similar to MF, RO also plays a major part in the implementation of AI-based models in predicting system performance. However, most of the AI models developed for the RO process have been ANN models, except for the RBF model proposed by Iranmanesh et al. (2016). In this study, an RBF model was developed to simulate an RO membrane system for use with desalination. A significantly high accuracy was observed in prediction of the water flux, with an R^2 value of 0.9997 and a MSE of 0.0009. This finding showed that RBF could be an accurate method for simulating RO performance. The remaining studies investigating prediction of the RO process focus on water permeability. Rajabzadeh et al. (2012) concentrated on the development of an ANN for the prediction of RO performance in the recovery of nutrients from biomass leachate. A R^2 of 0.99 and mean absolute percent error of 2.65% were observed for water flux simulation. ANN models for the estimation of water flux have been developed by several research groups worldwide (Barello et al., 2014; Farahbakhsh et al., 2019; Libotean et al., 2009; Madaeni et al., 2015; Salgado-Reyna et al., 2015), resulting in a maximum R^2 value of 0.996 and a minimum RMSE of 1.59 LMH, indicating that the developed ANN models may contribute greatly to optimizing designs of RO membrane processes in the future.

4.2. Osmotic-pressure driven membrane processes

Recently, forward osmosis (FO) (Figure S2, supplementary material) has attracted increasing attention in the fields of desalination and wastewater treatment and reuse. FO demonstrates significant benefits over pressure-driven processes, including the relatively low energy consumption, low propensity for fouling, and the production of high quality permeate (S.-J. Im et al., 2020). Many reports have described the use of FO in the treatment of wastewater such as medical wastewater (Lee et al., 2018), acid mine drainage (Vital et al., 2018), biological effluent (Boo et al., 2013), and activated sludge concentration (OMBR) (Viet et al., 2020).

The use of FO for water and wastewater treatment was proposed relatively recently, and the application of AI-based models in FO systems is therefore still rare in the literature (Table 3). Jawad et al. (2020) first developed an ANN model along with a multiple linear regression (MLR) model for the simulation of permeate flux during the FO process. The predicted results showed that ANN model demonstrated much higher performance

Table 3. Application of AI-based models in osmotic pressure driven and thermal driven membrane processes

| No. | Membrane processes | Type of AI model | Inputs | Dataset | Data preprocess | Output | Model performance | Implications | Ref |
|-----|--------------------|------------------|--|------------------------------|---|--|--|--|------------------------------|
| 1 | FO | – ANN – MLR | – Membrane type – Membrane orientation – FS, DS concentration – FS, DS CFV – FS, DS Temperature – Type of DS | 709 data points | – | Water flux | – ANN: $R^2 = 0.97$; – MLR: $R^2 = 0.51$. | – ANN is highly potential for prediction of water flux in the FO process. – ANN demonstrates a better performance than MLR. | (Jawad et al., 2020) |
| 2 | FO (OMBR) | – ANN – ANFIS | – MLSS, DO, EC, Time | 4 different datasets | Input data were randomized in the range of 0.1 to 0.9 | Water flux | – ANN: $R^2 = 0.94$, 0.98 and RMSE = 0.40, 0.14 for TFC and CTA – ANFIS: $R^2 = 0.98$, 0.99 and RMSE = 0.25, 0.12 for TFC and CTA membrane, respectively; | – Mixed liquor EC was shown to be the most important parameter. – ANFIS models demonstrating better prediction strength than ANN. | (Hosseinizadeh et al., 2020) |
| 3 | FO (OMBR) | RNN | – Water flux, conductivity | 100 data points | Normalization | – Water flux – Conductivity | RMSE of 2–3% | Deep learning is feasible for application in predicting OMBR water flux and salinity build-up | (Viet et al., 2021) |
| 4 | MD | ANN | – Parameters (flux, module design, temperatures, etc.); Membrane parameters (membrane porosity, thermal conductivity, pore size) | 240 experimental data points | Uniform distribution by Monte-Carlo approach | – Permeate flux – Outflow temperature | NNs have median errors, on average 20 times lower than Schofield and Modified-Schofield empirical methods. | ANN plays a vital role in guiding the derivation of new empirical methods. | (Dudchenko & Mauter, 2020) |
| 5 | MD (VMD) | ANN | – Pollutant type, feed temp., permeate temp., permeate pressure. | 25 samples | – | Permeate flux | $R^2 = 0.975$, MSE = 1.83. | The developed ANN model can predict the permeate flux in MD process with desirable accuracy. | (Dragoi & Vasseghian, 2020) |

compared to MLR, with R^2 values of 0.97 and 0.51, respectively. The model developed in this study provides opportunities for the simulation of FO related membrane processes, including OMBRs. Hosseinzadeh et al. (2020) constructed an adaptive network-based fuzzy inference system (ANFIS) and an ANN model for forecasting water flux in an OMBR system (Hosseinzadeh et al., 2020). However, in this study, MLSS, dissolved oxygen (DO), electrical conductivity (EC), and time were input as datasets without preevaluation. The predicted results indicated that ANFIS models demonstrate a better prediction strength than ANN, with R^2 values of 0.98 and 0.94 (in TFC), respectively and R^2 values of 0.99 and 0.98 (in CTA). The lowest observed RMSE was only 0.12, which was from the water flux prediction using the CTA OMBR process with ANFIS. Similarly, Viet et al. (2021) performed an RNN model for the prediction of water flux and conductivity in the long-term operation of an OMBR system (S. J. Im et al., 2021; Viet et al., 2021). The study reported a predicted water flux with a difference of less than 3% between the actual and the simulated data, implicating that AI-based models are effective in predicting the system performance of FO, not only as a standalone process but also for integrated processes such as OMBR (Viet & Jang, 2021).

Even though models have been developed for FO process, the existing articles have focused the most in prediction of water flux and reverse salt flux. There are dozens of works need to be considered in future for enhancement of overall FO systems, such as estimation of membrane fouling, energy consumption, or even the life cycle of membrane materials. Several specific recommendations for future studies will be discussed in the later section.

4.3. Thermal-driven membrane processes

Membrane distillation (MD) is a thermally driven membrane separation process. In MD, water is transported as vapor across a hydrophobic microporous membrane from the feed side to the permeate side under a partial vapor pressure gradient. Because the performance of MD does not depend on the salinity of the feed solution (even at levels such as 200,000 ppm), it is considered a promising and cheaper alternative to RO.

Four main types of MD can be distinguished from the strategies that are used to collect the vapor transported from the feed to the draw side: direct contact MD (DCMD), air gap MD (AGMD), vacuum MD (VMD), and sweeping gas MD (SGMD), as shown in [Figure S3, supplementary material](#). All four types of MD have been applied in such fields of study as the desalination of seawater and brackish water, the treatment of oily wastewater,

the food and beverage industries, animal husbandry, the concentration of acids, and mineral recovery.

Similar to FO processes, the application of AI-based models to thermal-driven MD processes has been limited in previous studies (Table 3). The physical parameters in the MD process were predicted by Dudchenko and Mauter (2020). In this study, the dataset is not an actual set, but is instead a simulated set created by heat and mass transfer models (via empirical methods), which may reduce the accuracy of the model when it is applied to actual MD processes. A lower median error was observed in the NN models than that obtained using Schofield and Modified-Schofield empirical methods. However, NNs still did not fit the experimental dataset; this is because NNs cannot solve the challenges associated with random error in the data. The black box used in NNs also cannot ensure that the estimation is meaningful when used in real experiments. Thus, the authors suggest that NNs should not be used as a replacement for empirical modeling strategies. It seems NNs require further investigation to enhance their performance in the prediction of MD processes. Although the accuracy needs attention, the developed ANN models for the prediction of permeance using VMD will likely produce remarkable results in the future simulation of MD processes.

Application of AI-based models in thermal membrane processes is still rare so far. The complexity as well as novelty of this process may be the major reason for that. This should be taken into consideration by researchers worldwide, especially in simulation of energy consumption as well as the potential of applying renewable energy in MD process, then contributing to reduction of total operating cost and enhancement of system performance. More discussion on future perspectives of AI application in MD will be presented in the later section.

5. Implications and future prospects

5.1. Implications

The high performance of AI-based models that are applied to membrane processes for desalination and wastewater treatment implies that AI technology is feasible for predicting non-linear relationships in treatment processes, which is very difficult to achieve with conventional mathematical models. Figure 4 shows that the average performance of AI-based models is much higher than that of mathematical models. The AI tools demonstrated a narrow variance with a high R^2 value that ranged from 0.98 to nearly 1.00 and a mean value of 0.99 while conventional models vary over a broad range from 0.92 to 0.98 in terms of these parameters, with a mean value of above 0.96. The result implies that novel AI tools are much more

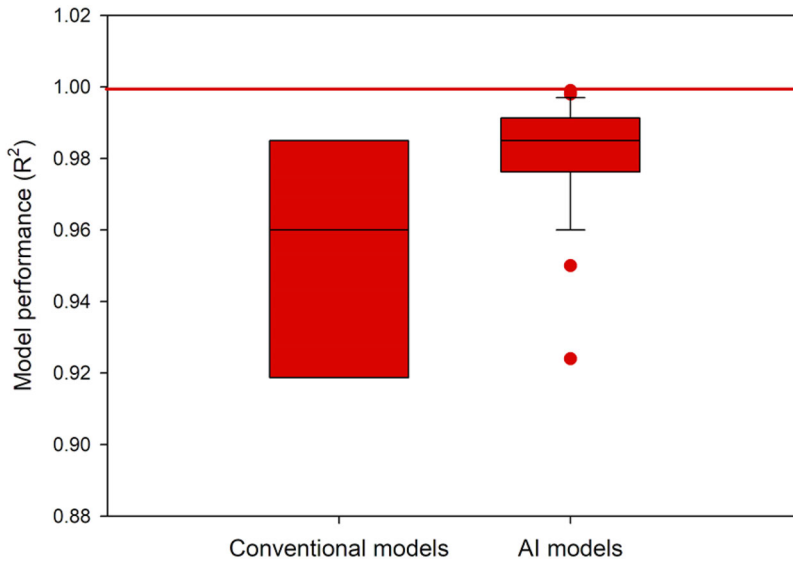


Figure 4. Comparison of the performance of AI-based models with that of conventional models.

beneficial than conventional mathematical models, not only in terms of the convenient process of model development and performance (as shown in Sec. 3.2) but also in the high accuracy of the predicted results.

In addition, the models are not only able to simulate the water flux, but also the removal efficiency, membrane fouling, and even membrane fabrication for all membrane processes, including pressure-driven, osmotic pressure-driven, and thermal-driven systems, which seems impossible to be performed well by conventional models. AI models also provide a novel strategy that can be used to further understand the complicated phenomena that occur in membrane water treatment processes, strongly supporting the decision-making process in actual systems. Therefore, the optimization and design of these membrane processes is expected to be easier and more effective than ever over the next few decades. The successful application of AI-based models in membrane processes for water and wastewater treatment therefore provides many opportunities for the enhancement of environmental systems in the future. Several suggestions for future works have been therefore included in the next section.

5.2. Recommendations for future studies

The application of AI-based models to membrane processes was proposed relatively recently; therefore, various fields surrounding this topic still need to be addressed in the future.

5.2.1. Improving model performance

1. Increasing the size of the dataset: Current studies investigating on AI models utilize datasets that are collected from several studies or from a single experiment, which release a small and local set of data. AI methods require a large dataset for the overall training and validation of models. Further exploration into the size of the dataset and its effects on model performance is necessary to enhance the model performance.
2. Enhancing the representative dataset: As indicated previously, almost datasets used are currently obtained from a local plant or collected from different studies, resulting in the use of non-representative datasets for model training, which may reduce the feasibility of applying AI-based technologies in real treatment plants in the future. A systematic experiment should therefore be conducted under various operating conditions to obtain a sufficient and representative dataset for the development of models.
3. Development of hybrid AI models: Although single AI tools have demonstrated good enough performance, hybrid AI technologies so far appear to be able to increase the simulation performance.
4. Development of new algorithms (i.e., new AI tools): The membrane system has been developed continuously; consequently, the operating parameters and input sets used for modeling will change accordingly. If the current models are not updated, the model accuracy will be reduced, and the processes cannot be simulated well. The evolution of new AI tools could be an effective way to tackle these problems in the future.
5. The combination of AI technique and conventional mathematical models: As discussed previously, though AI models is very effective in simulation of membrane system performance, it is not very suitable in some cases that we need to take a deep understanding on the process' mechanism, while this could be done easily by mathematical models (but with lower accuracy). Therefore, it is very interesting to investigate the integration of AI tool in adjustment of certain parameters of conventional models in order to describe process in a more effective simulation.

5.2.2. Model application in membrane processes

1. Prediction of other operating parameters: Recent developments in the use of AI-based models with membrane systems have provided an effective prediction of membrane filtration performance, such as water flux, salt flux, and the removal of contaminants. However, other operating parameters that are involved in membrane processes require simulation, such as changes in the membrane properties following operation,

or the life span of a membrane used in water and wastewater treatment systems. Membrane fouling, in particular separately reversible and irreversible fouling formation have not been investigated yet. In this field, the AI models seems very effective in prediction of these fouling layers; it can suggest solutions for preventing the fouling formation by control the dynamic parameters, reducing total operating cost.

2. Application of AI models with other types of membrane: In addition to pressure-driven, osmotic pressure-driven, and thermal-driven membrane processes, other types of membrane are also applied in water treatment, such as electrodialysis (ED) and emulsion liquid membranes (ELM). To the best of our knowledge, no studies on the application of AI technologies have been conducted that investigate the simulation of the performance of these membrane systems. Thus, it is beneficial to simulate these processes using AI technology.
3. The application of AI to hybrid membranes: Although there are several applications in which AI-based tools have been used with hybrid membrane systems such as RO-NF, MBR, and OMBR, many important hybrid systems still require simulation. Predicting the various operating parameters included in these hybrid processes may provide information that can be used for better control of these systems in the future.
4. The membrane processes with AI play an indispensable role in adaptation to global challenges: AI is able to not only enhance the membrane system performance but also demonstrate dozens of potential benefits. For example, integrating AI to membranes may contribute to reduction of greenhouse gases (GHG) emissions by optimizing the system (i.e., reducing the waste discharge) and maximizing the life-cycle of materials. The hybrid AI-membranes may also increase the suitability of membrane processes in application to treatment of various types of wastewater in the future. These capabilities should be paid attention in the future research.
5. Finally, the integration of AI tools in real membrane-based wastewater treatment plant (WWTPs): Most of the current AI-based models describing membrane processes have been conducted for scientific research owing to the novelty of this field. To produce an automatic control system in real membrane-based WWTPs, studies connecting AI tools with actual processes are necessary. This investigation may require interdisciplinary research by environmental scientists together with information technology engineers and automation scientists. AI models will need to be integrated into platforms, sensors, and communication networks to produce automatic predictions and recommend actions or decisions for maintaining and enhancing the performance of a membrane system. Thus, the control systems can be enhanced for better and

more timely decisions as well as maximized revenue capture and produced water quality.

6. Conclusions

In this study, AI-based models simulating the membrane processes used in sustainable water and wastewater treatment were critically reviewed.

- Existing mathematical models used for membrane processes and their advantages and disadvantages were emphasized.
- The theory and classification of novel AI tools in the simulation of membrane processes were presented and the benefits of using AI models over conventional mathematical models were critically indicated.
- The current membrane processes and recent applications of AI-based technologies in these membrane separation systems were thoroughly discussed with the aim of providing audiences with state-of-the-art tools for membrane system simulation.
- The implications of the review and suggestions for future research into the application of AI-based models to membrane systems were demonstrated.

AI technology is expected to create a breakthrough in the control and enhancement of environmental systems, and in particular membrane processes, by providing us with actionable insights to produce fit-for-future systems, which may bring us closer to smart cities in the context of sustainable development.

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