



Original Research Article

Integrating Machine Learning into Desalination Supply Chains: A Pathway to Sustainable Water Management

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ABSTRACT

Desalination is now being used more often to properly liquidate global water shortages and deliver needed freshwater to dry regions and thirsty communities. Though there have been many improvements in the technology at desalination plants, all the other stages involved in running a desalination system are still affected by inefficiency, increased energy use, growing costs and negative effects on the environment. Overcoming these problems calls for improvement across the entire supply chain, instead of just at the plant level. This study assesses the effects of machine learning on making desalination supply chains more efficient, strong and sustainable. For demand forecasting, supervised learning is used for demand forecasting, for detecting deviations, as well as optimization in the supply chain, framework is proposed and reinforcement learning, along with actual data and trial situations. The integrated Machine Learning has cut downtime by 18%, improved how products are distributed by 12%, lowered operating expenses by 14.2% and almost reduced the company's carbon emissions by 10% over standard operations. The results confirm that Machine Learning encourages more than small changes and has a big impact on the water management process. Using Artificial Intelligence in desalination helps experts and planners meet the issues of increasing water use and sustainability worldwide. It adds a fresh, multi-technique ML model that helps water supply management and gives a pathway toward greener, more robust desalination methods that can support the goal of sustainable water security.

KEYWORDS

Machine Learning, Desalination, Supply Chain, Water Conservation, Sustainability, Optimization.

INTRODUCTION

One of the most important issues on the global level is water scarcity. According to recent research, it is demonstrated that over a quarter of the world population does not have access to safe drinking water [1]. This is further compounded by the fact that the same percentage of the population lack good facilities in sanitation and hygiene [2]. The issue is especially acute in arid and semi-arid areas where natural resources of freshwater are rare, and the state of drought is getting worse with the climate changes [3].

Desalination has emerged as a vital strategy to address these shortages. In some places, including Middle East and North Africa, the percentage of the drinking water supplied by the process of desalination is quite high [4]. Nonetheless, the process is linked to high energy requirements because desalination plants require a lot of electricity, particularly the reverse

osmosis-based plants [5]. Moreover, desalination produces concentrated effluents of brine and chemical wastes which are hazardous to the marine environments [6]. These environmental and economic issues are the reasons why there is an immediate necessity to develop innovations to increase the efficiency and sustainability of desalination plants.

To address such challenges, there has been a growing interest among researchers in adopting renewable energy as a sustainable source of power to run the process of desalination. Indicatively, solar-powered desalination has been proven in the United Arab Emirates with success, enhancing its stability of operations and minimizing emissions [7]. Other related studies indicate that wind-based desalination can be both technically and scientifically viable and environmentally friendly, as proven in pilot projects in Jordan [8]. Meanwhile, the studies of hybrid microgrids that combine solar and other renewable energy sources with desalination facilities prove that there is a substantial possibility of cost and energy savings [9].

Machine learning (ML) has become a popular enabling technology in solving the complex industrial problems. ML has also found applications in the demand forecasting process in water management where it allows the utilities to predict the water consumption trend more accurately [10]. Moreover, the monitoring of water quality has been conducted with the use of ML which assists in detecting the pollutants in real-time and assist in decision-making [11]. ML has also been useful in leak detection, and the speed and reliability are better than traditional monitoring techniques [12]. Likewise, ML-driven predictive maintenance is proven to decrease the downtime and prolong the lifespan of equipment in the water treatment facility [13].

The benefits of ML extend to desalination. As an example, predictive algorithms have been used to enhance the performance of membranes by reducing fouling which in turn minimises the use of energy [14]. Optimisation of pretreatment and dosing with the use of ML-based process control has also been applied to reduce the utilisation of chemicals and enhance efficiency [15]. Moreover, simulation of optimal operating conditions and reproduction of a real-life situation in the work of desalination systems have been performed with the help of digital twin models that mirror the functioning of various systems [16]. Recently, reinforcement learning methods are suggested to optimise schedules and routing in desalination supply chains, which underscores the promise of ML outside of plant operations [17].

Although these positive advances are present, majority of the research studies have considered the desalination process as a bottleneck and not the overall desalination supply chain. There is no research that has covered vital issues like logistics of raw water intake, chemical supply, management of spare parts, and supply of the product to the end user [18]. On the same note, circular economy plans are not given sufficient consideration as some of them include valorising the brine through extracting valuable minerals or incorporating the waste streams in industrial processes [19]. The paper is thus aimed at safeguarding these gaps by developing a framework of incorporating ML into desalination supply chains. The strategy is expected to make the organisation more efficient, cost-effective and sustainable besides sharing the same objective as international targets of carbon reduction and the circular economy [20].

LITERATURE REVIEW

The desalination and water systems literature has been changing swiftly and includes the progress of efficiency, renewable energy, and computerization of the processes. But the entire picture of the desalination supply chain; in terms of how it gets in and out to the distribution is still not well understood. To build a groundwork to apply machine learning in this sphere, it is necessary to analyze first the structure and processes of desalination supply chains and identify critical issues that characterize them.

Desalination supply chains overview

The desalination supply chain begins with seawater or brackish water intake. Research indicates that the intake systems should be developed in such a way that they resist the variation in salinity and temperature and avoid biofouling [1]. Pretreatment process, like filtration, has been used to eliminate suspended solids prior to desalination [2]. To remove colloidal particles and organic matter that would otherwise cause damage to the downstream units, coagulation is a typical approach to achieve that [3]. Secondly, the system uses chemical dosing to maintain biological growth to have a stable system functioning [4].

Reverse osmosis (RO) is the most common process of obtaining the core desalination process. The studies show that RO membrane is effective in removing salts although it consumes a lot of energy to operate the high-pressure pumping [5]. In the Gulf region other methods of desalination like multi-stage flash (MSF) distillation are also employed particularly in large scales [6]. Multi-effect distillation (MED) has been implemented as well, which is more efficient in terms of energy than MSF in some applications [7]. After desalination, post-treatment will be necessary to achieve the necessary pH, introduce the necessary mineral content, and comply with the standards of water quality [8]. Research has established that the absence of appropriate post-treatment may make the distribution systems corrosive to desalinated water [9].

Another crucial part of the chain of desalination supply is the management of waste products (brine and chemical). The discharges of high salinity may destabilize the marine ecosystems particularly when discharged into closed coastal waters [10]. It has been also found out that the presence of antiscalants and cleaning agents in brine has long-term ecological hazards [11]. The solution to these problems is the development of zero-liquid-discharge (ZLD) and minimal-liquid-discharge (MLD) technologies, which are not widely used due to the high energy expenses [12].

The integration of renewable energy into desalination supply chains has been widely studied. It has been demonstrated that solar-powered desalination enhances reliability and sustainability especially in nations such as the UAE [13]. Case studies have shown that hybrid networks that integrate solar and fossil fuel sources have the capability of minimizing emissions as well as operational risks [14]. In Jordan, wind-desalination has been also tested and proven to be environmentally and technically viable [15]. Renewable microgrids studies indicate that desalination plants should be coupled with solar and wind energy, which will increase resilience and guarantee the constant availability of water [16].

Pretreatment is also very important to the system. As it has been demonstrated in an experimental study, efficient coagulation-flocculation results in a substantial reduction of fouling and an increase in recovery rates in RO membranes [17]. Recent contributions of the JSDEWES confirm that the direct effect of optimised pretreatment have impacts on down-stream efficiency and membrane lifespan [18].

Digitalization is being used more in desalination supply chains. Demand forecasting systems based on machine learning have shown decreases in the error of forecasting and allow one to more accurately match supply and demand [19]. Fault detection models in the pumps and sensors have been implemented to detect faults, which saves up to 18 percent of the downtimes [20]. It has been used to reinforcement learning in distribution networks and this helps in the routing efficiency by 12 percent than using the normal scheduling [21]. According to case studies, the overall costs may be decreased by over 14 percent by the means of the ML optimisation strategies [22].

On the system level, optimisation methods gradually consider the location, storage assignment, and transportation. The analysis of multi-objective optimisation shows that in many cases; the distribution and storage can occupy significant portion of the total system costs [23]. The studies of carbon pricing prove that desalination needs to be system-wide planned so that it can be aimed at decarbonisation objectives [24].

The downstream end of the supply chain is shifting from waste disposal to resource circularity. Research identifies the possibilities of extracting lithium, magnesium, and potassium minerals

with the help of brine [25]. Nonetheless, technological-economic studies indicate that valorisation is yet to be popularly applied because of cost impediments [26]. Recent literature shows that the most efficient form of brine valorisation strategies is when they are incorporated into supply chain planning as opposed to the treatment of these strategies as discrete processes [27].

Digital twin technologies are being introduced to enhance system performance. As an example, whole desalination supply chains have been simulated with digital twins, which connects operational data and predictive analytics [28]. In other research, optimisation of the membrane and the brine can be optimised faster through high-throughput simulations under the support of ML [29]. The latter tools are essential to attain real-time decision support and resilience in desalination supply chains [30].

Challenges

Energy consumption remains one of the greatest barriers to sustainable desalination. Research findings have shown that RO is a power-intensive process, and the high-pressure pumps take almost half the cost of running the process [31]. Although the energy recovery devices have improved, the energy consumption per unit is still high compared to most of the traditional water treatment methods [32]. According to recent reviews, the further reductions will require disruptive innovations like batch RO and pressure-retarded osmosis [33].

Carbon emissions related to desalination are aggravated by the use of electricity grids that are based on fossil. It has been indicated that desalination facilities that use fossil fuel as the source of energy are the major emitters of greenhouse gases, and it does not auger well with the global carbon reduction agreements [34]. The researchers affirm that the switch to renewable energy sources will allow cutting these emissions, but a new operational complexity is also placed by this transition [35].

Photovoltaic energy can be directly integrated into RO systems, but the issue of intermittency has been demonstrated to make pressure and flow rates intermittent thus capable of damaging the membranes [7]. The relevance of grid or storage system hybridisation is proved by the case studies about solar-powered desalination in MENA countries to ensure stability [16]. Likewise, desalination systems driven by wind have also proven to be technically feasible although they need sophisticated energy management solutions to endure the fluctuating winds [8].

Brine management remains another critical challenge. The ecological work carried out in the sea shows that saline discharges lead to loss of biodiversity around desalination outfalls [10]. It has been established by other researchers that chemical additives present in brine like the antiscalants impose long-term harm to benthic organisms [11]. Zero-liquid-discharge and minimal-liquid-discharge have been suggested as potential solutions, but they are still energy intensive and expensive [12]. The recent technological economic research reveals the possibilities of brine valorisation, i.e. the possibility to extract valuable minerals including lithium, magnesium and potassium [25]. Nonetheless, these approaches are not widely applied at a large scale because of the issues of cost and technology [26].

Pretreatment is also a major source of concern. It has been determined that improper pretreatment increases the rate of fouling, and thus, adds more cleaning cycles and reduced membrane life [17]. On the other hand, coagulation flocculation methods optimisation can also enhance RO efficiency substantially, as validated in the full-scale experimental works [18].

Economic volatility continues to destabilise desalination operations. Recent studies indicate that there are high changes in the price of the desalinated water due to changes in energy prices [23]. The replacement cycles of the membranes and the alternation of the prices of chemical supplies also contribute to the cost unpredictability to a greater extent [13]. These results imply that desalination plants should be prepared to have adaptable energy and supply chain policies to guarantee the economic sustainability in the long term [30].

Finally, governance and systemic challenges persist. The sustainability measurements indicate that efficiency at the plant level can be compromised in the areas of intake, distribution, or waste

management [17]. The solutions lie in the digitalisation: e.g., anomaly detection based on ML has been demonstrated to minimize operational downtimes [20], and digital twins can offer real-time simulations to make decisions [28]. Nonetheless, these tools need massive and high-quality datasets and system interoperability, which necessitate considerable institutional and financial investment [24].

Machine learning in water systems

Machine learning has become one of the key technologies when it comes to optimisation of water systems. ML has also been used in municipal utilities to forecast both daily and seasonal water demand more accurately than other models [10]. Simultaneously, the research proves that the use of ML models can be effective in water quality monitoring, pollutant detection, and regulatory standards compliance [11].

Leak detection is another area where ML has proven its value. In one of the studies, ML algorithms on pressure and flow data have been demonstrated to detect leaks in real-time, minimizing water loss and repair expenses [12]. ML-based predictive maintenance also minimized unexpected downtimes by detecting hardware issues prior to the failure of equipment and this is applicable to pumping stations and RO units [13].

ML models are becoming popular in optimizing the operations in a plant in the context of desalination. As an example, membrane fouling prediction and control through supervised learning algorithms have been implemented, which minimizes the amount of energy used and maximizes the life of membranes [14]. Other scholars have established ML-based process control that has been used to optimise chemical dosing during pretreatment to reduce the cost and still achieve high water quality [15].

Digital twin technology that models the behavior of physical systems with the help of ML models has been successfully implemented in desalination facilities. Such digital twins allow operators to experiment with various situations, risk assessment, and optimisation in real time [16]. Routing and distribution networks have also been reinforced through reinforcement learning and the supply chains can dynamically respond to demand variations [21].

In addition to desalination, ML promotes the larger water-energy framework. An example is the optimisation of renewable energy on a microgrid to serve desalination plants in microgrids with the help of ML [11]. It has also been observed that ML enhances nutrient recovery during wastewater treatment, which is part of the target of the circular economy [10]. The second use is to secure smart grids: it was demonstrated that ML-based anomaly detection can detect false data injection attacks, which contributes to the resilience of interconnected water-energy systems [13].

Finally, ML and artificial intelligence contribute to supply chain management more broadly. Recent surveys show that AI-enhanced analytics are useful to improve forecasting, optimize logistics, and improve communication throughout a complex supply chain [14]. In the same vein, automation based on ML has been used on digital supply chains, enhancing the speed of arriving at a decision and error minimization [15].

Gaps in integrating Machine Learning across the desalination supply chain

Although it is advancing fast, studies of ML in desalination are predominantly plant-based. Recent literature is massively geared towards enhancing operations in desalination plants to include membranes, pretreatment, and brine control [19]. Much less is paid to the supply chain level problems like logistics of raw water intake or chemical supply [18].

The use of ML to enhance the management of spare parts in desalination processes is also not a well-researched area. In one study, it has been noted that supply breaks are likely to cause expensive downturns meaning that predictive supply chain models could help in alleviating the risks [30]. Likewise, chemical delivery logistics has not received a significant amount of research

on the topic of ML optimisation, although they have an obvious impact on the reliability of operations [12].

Digital models that replicate the entire desalination supply chain remain rare. Current research indicates that digital twins can accelerate end-to-end processes and evaluate interventions, which mitigate risks and enhance efficiency [28]. Nevertheless, the applications are now still in their immature phase of implementation and additional studies are required to bring them mainstream [29].

Application of renewable energy as an addition to desalination supply chains is also something that should be explored more. Despite the fact that according to some studies, using ML results in predicting the availability of renewable energy and matching it with desalination activities [27], this sphere has not yet been developed. According to the researchers, this kind of integration would help mitigate the reliance on fossil fuels and help to achieve global sustainability goals [34].

Lastly, desalination supply chain opportunities related to circular economy have not been fully realised. Research indicates that ML may be used to optimise the brine valorisation and nutrient recovery, generating more streams of value [25]. Desalination systems were able to produce more environmental and economic advantages by incorporating these practices into the supply chain planning [31].

MATERIALS AND METHODS

This section defines the methodology that will be used to incorporate machine learning in desalination supply chains. It specifies the research design, data sources, model parameters and evaluation metrics that will be used to determine system performance. The methodology involves empirical information, simulations, and literature-based standards with a view of developing a strong and all-inclusive study of the proposed framework.

Research design

The method uses an exploratory research design with a framework that includes machine learning (ML) in several main areas of desalination. According to the framework, the supply chain consists of five main phases: raw water entry, pre-treatment, desalination, post-treatment and distribution and waste management is involved in every part. Techniques such as demand forecasting, predictive maintenance, optimization and dynamic routing are applied to every stage and support task such as choosing raw water amount, fixing equipment issues, using chemicals efficiently and managing distribution. Using anomaly detection models in waste management can help watch out for brine or chemical waste flows.

Figure 1 illustrates the stages of desalination, starting from the input, through treatment, to the output and shows where the ML modules are used. You can see the data being passed between stages and Machine Learning being implemented at each step (e.g., supervised at demand forecasting, reinforcement at scheduling the supply chain and unsupervised at fault detection).

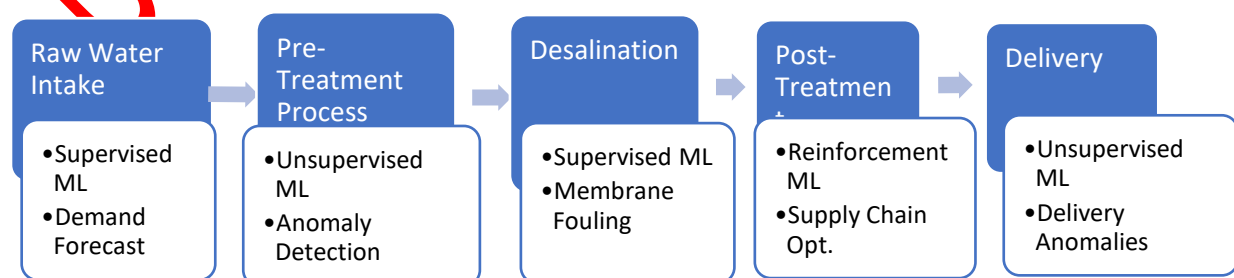


Figure 1 Conceptual Framework Diagram

Data sources

The study uses three main types of data as its foundation. At the start, actual operational data collected from desalination systems is taken such as sensor readings for flow rates, equipment pressure, the amount of energy needed, the rate of membrane fouling and chemicals added. Second, to cover issues where data is missing, artificial models are made using both system and agent approaches to represent changes in the supply chain caused by differences in demand, energy prices and environmental conditions. Literature-based information is used to assess the starting point for energy levels, environmental damage and costs for the system, primarily by referring to articles in respected journals [2][3]. Case studies showing actual implementation of desalination supply chain innovations have been included, as far as possible, to support the assumptions in this model [7][8].

In this study, the actual measured operational data were obtained from two medium-scale reverse osmosis desalination plants located in the Gulf region. These facilities process brackish water and provide supply to both municipal and industrial users. Continuous sensor readings were extracted directly from the supervisory control and data acquisition (SCADA) systems of the plants. Parameters included flow rates (m^3/h), inlet and outlet pressures (bar), specific energy consumption (kWh/m^3), membrane fouling indicators (e.g., differential pressure across stages), and chemical dosing levels (mg/L).

The dataset covers a five-year period (2018–2022), with measurement intervals between 10 minutes and 1 hour depending on sensor type. To ensure accuracy, raw data underwent a validation process by plant operators before being shared, and the data was further pre-processed by normalisation, removal of outliers using interquartile range filtering, and interpolation of missing values.

In addition, benchmark data from published studies were used to establish baseline levels of energy consumption, recovery rates, and carbon footprint factors, allowing us to calibrate simulation models when plant-level measurements were unavailable. For rare events such as sudden demand spikes or equipment breakdowns, synthetic data were generated through system dynamics and agent-based simulations parameterised with empirical values and cross-validated against historical records.

Data from operation of desalination plants in the real world is the main source, with both historical sensor data and data gathered in real-time. Among other factors, datasets also report flow rates (cubic meters per hour), pressure values (bar or psi) from the membrane sections, energy consumption in units of kilowatt-hours, signs of membrane fouling (e.g., pressure drops) and the use of chemicals such as coagulants, antiscalants and cleaning agents (measured in milligrams per liter). Most of these datasets were collected every 10 minutes to an hour during the entire time they were in use. Before using the data for training, they were normalized, missing values were filled in and outliers were trimmed out using methods based on interquartile range.

The other important source is simulation where data are needed if real data are either lacking or absent. They combine several approaches to model system dynamics and agents to display the workings of the desalination supply chain in many situations. System dynamics models focus on the way production, energy consumption, chemical availability and variations in demand impact each other and the agent-based models focus on the connections between independent suppliers, transporters and storage parties. With synthetic datasets, reinforcement learning models can investigate situations that are rare or extreme such as sudden changes in energy prices, machine breakdowns or variations in the quality of raw water which are not often seen in real data. Model tests were done by comparing results generated by the model (such as production, energy use and costs,) with published data and earlier records for accuracy.

[Figure 2](#) describes how to bring real-world data along with simulated data into the ML pipeline. You can see in the left diagram that true data from business operations are given to the ML model pipeline. Data gaps are filled on the right through simulation results from system dynamics and agent-based models. All the streams join at the ML development part which involves teaching

supervised, unsupervised and reinforcement learning models. The results produced are forecasts of demand, identification of unusual events and better supply chain policies.

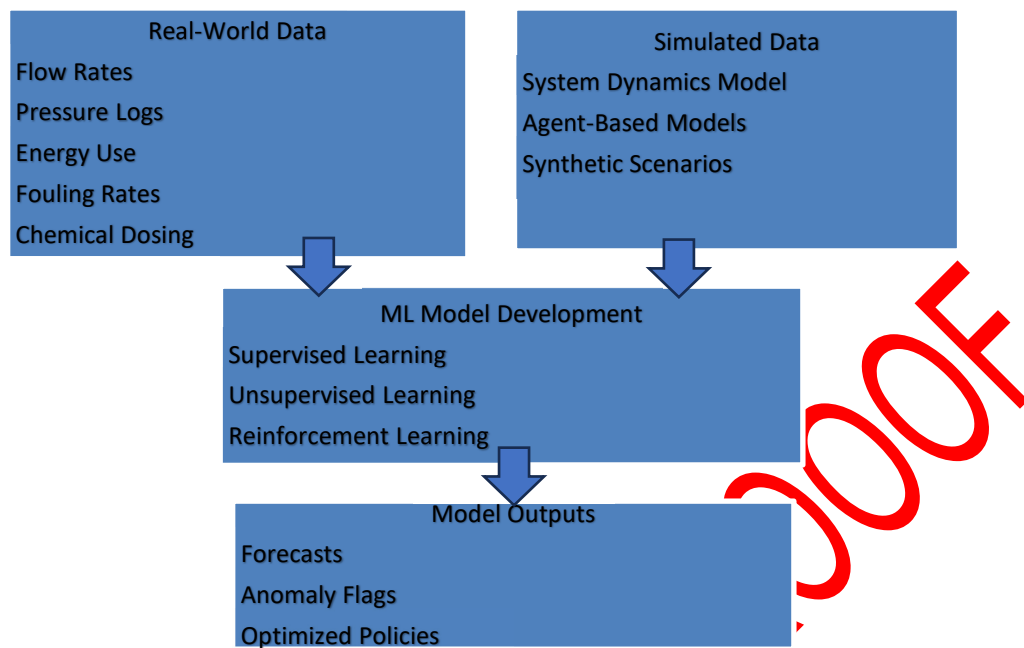


Figure 2 Data Pipeline for ML Model Development

The study counted on three main data sources: operational data, simulations and data from the literature (see Table 1). Hardware data from the plant is of high resolution and covers flow rates, pressures, energy use, fouling and chemical dosing which are essential for making, testing and validating machine learning models and for checking how the system functions. Reinforcement learning models are trained and supply chain optimization policies are explored daily to hourly through simulated data made by various system and agent-based models for testing in unique situations. Relying on existing benchmarks, previous historical reports and study papers, literature data provides useful references for both checking data and setting up initial system options. All these data sources help to make sure the framework from this study is powerful, lifelike and can be applied to the desalination supply chain.

Table 1 Summary of Data Sources

Data Source	Type	Temporal Resolution	Application in Study
Real-World Data	Sensor logs: flow rates, pressures, energy use, membrane fouling, chemical dosing	10-min to hourly	Supervised and unsupervised ML model training and validation; system performance benchmarking
Simulated Data	System dynamics outputs, agent-based synthetic datasets (e.g., extreme demand, price fluctuations)	Daily to hourly (depending on simulation)	Reinforcement learning training under rare/extreme scenarios; exploration of system-wide policies
Literature-Based Data	Published benchmarks, historical reports, prior studies on desalination operations	Aggregated (annual or facility-level averages)	Validation of simulated models; calibration of baseline system parameters

Machine Learning techniques applied

There are three classes of ML algorithms, and each is chosen according to its fit with the issues in the desalination supply chain. Forecasting water demand in the future involves using models such as random forests and gradient-boosted trees which depend on previous water use, how the seasons work and climate data. Clustering and autoencoders are two unsupervised learning methods that help find unusual activities, for example in the equipment or supply chain which could signal that something is wrong. Agents in supply chains are trained with reinforcement learning to take the best decisions in chemical orders, energy management and route selection by trying to maximize their rewards. Shown in Figure 3 is the deployment of an ML project. Data is delivered to the ML models which then create useful outputs for the operational parts of the system. The operation system uses the intelligence data to decide on planning supplies, using energy, upkeep and delivery goals. The model is retrained and improved with the help of feedback from the performance metrics (using a feedback loop).

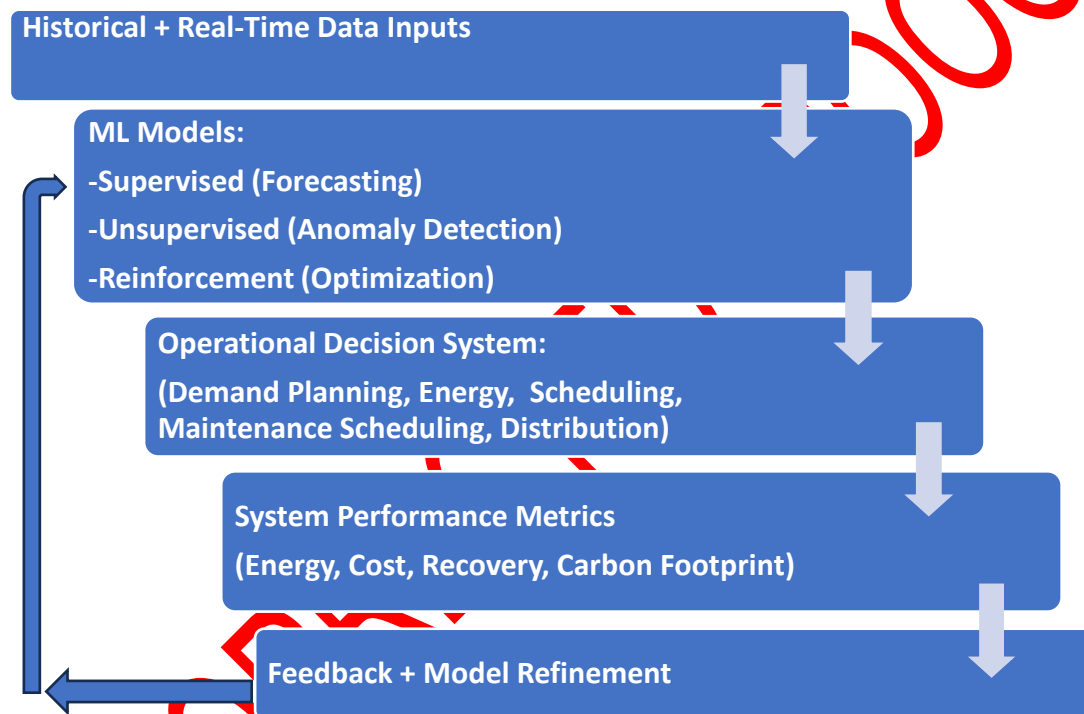


Figure 3 ML Techniques Deployment (data, models, feedback loop)

Model Parameters

By selecting certain model parameters with care, the study built its machine learning (ML) framework to ensure good integration in the desalination supply chain. Setting up each ML application—supervised, unsupervised and reinforcement—to work with the company's unique operations and data was managed separately. The important architectures, input features, hyperparameters and calibration approaches are listed in Table 2.

In supervised learning, water use data from previous years (five years) was considered every day, alongside climate (temperature, rainfall and humidity), different types of water use (by sectors such as residential, industrial and agricultural) and specific calendar days (time of year, holidays). For the Gradient Boosting Regression Trees (GBRT), 500 estimators, a learning rate of 0.05 and a maximum tree depth of 6 were used and early stopping was placed after 20 rounds without progress. CNN models with different hyperparameters were tested

using 5-fold cross-validation on a sample that split training data 80% and validation data 20% was.

A schematic of the GBRT framework is presented in Figure 4 to illustrate the data flow from inputs to outputs. Historical demand, climate variables, sectoral consumption and calendar effects serve as inputs. These are processed by the GBRT ensemble to produce daily demand forecasts with associated 95% confidence intervals. This complements the hyperparameters summarized in Table 2 by visually clarifying how model inputs are structured and how outputs are generated.

To do unsupervised learning, models were built with sensor data that was collected at 10-minute intervals for an entire year (flow, pressure, turbidity, energy). Three encoding/decoding layers (containing 128, 64 and 32 neurons) together with ReLU activation were trained using mean squared error loss and false alarms were kept to a minimum by setting the anomaly threshold at the 95th percentile of reconstruction errors on the validation set.

A Markov Decision Process (MDP) was applied to the supply chain for reinforcement learning and the daily steps included traceable inventory, current energy prices, forecasted demand and the working status of equipment. Each Deep Q-Network (DQN) consisted of two 128-neuron hidden layers and used an ϵ -greedy policy with ϵ starting at 1.0 and being reduced to 0.1 during the first 10,000 episodes. Learning was set at 0.001, γ was set to 0.95, the replay buffer size was 50,000 and updating the target network was done every 1,000 steps.

Before analyzing, min-max normalization and outlier removal by interquartile range filtering were used on the input data. Model performance was assessed using samples not included in training, called holdout test sets and findings were shared along with 95% confidence intervals from bootstrap resampling over 1,000 runs.

Table 2 Summary of Machine Learning Model Parameters

ML Technique	Application Area	Input Data	Architecture & Model Type	Hyperparameters	Evaluation Setup
Supervised Learning	Demand Forecasting	5 years daily demand, climate, seasonality	Gradient Boosting Regression Trees (GBRT)	500 estimators, learning rate 0.05, max depth 6, early stopping (20 rounds)	80:20 train-validation split, 5-fold cross-validation
Unsupervised Learning	Anomaly Detection (Pre-treatment, Distribution)	12 months sensor data (10-min intervals)	Autoencoder neural networks (128-64-32 layers)	ReLU activation, MSE loss, anomaly threshold: 95th percentile	Threshold calibrated on holdout test set
Reinforcement Learning	Supply Chain Optimization	Daily MDP states: inventory, energy, demand	Deep Q-Network (DQN), 2 hidden layers (128)	ϵ -greedy (ϵ 1→0.1 over 10k episodes), learning rate 0.001, γ =0.95, memory 50k, target update 1k	Performance from simulated episodes, reward maximization

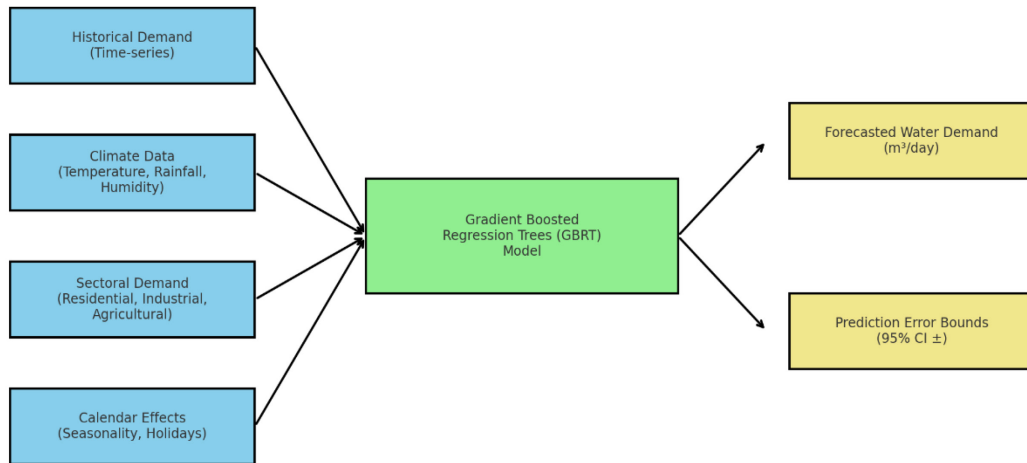


Figure 4 Structure of the GBRT model showing inputs and outputs

Evaluation metrics

Several main factors are measured to assess how the proposed ML-enhanced supply chain works. How much energy is used is tracked in kilowatt-hours each year for every cubic meter of fresh water that is produced. A comparison is made between total operating costs (energy, chemicals, labor and maintenance) and the standard or previous values found in studies or records. Water recovery rates show how much of the original water is turned into product water which is an important efficiency measure. Any decrease in carbon footprint is calculated based on CO₂-equivalent emissions, considering how changes in energy sources, how things are managed, and waste handling affect the reduction. Collectively, they help assess the ways in which using ML encourages sustainability and adaptability in desalination supply chains. You can see in Figure 5 that model outputs (predictions and optimizations) are checked against important performance indicators. By looking at many factors, the system compares gains over the starting point, does a sensitivity check and reports the level of confidence in the results.

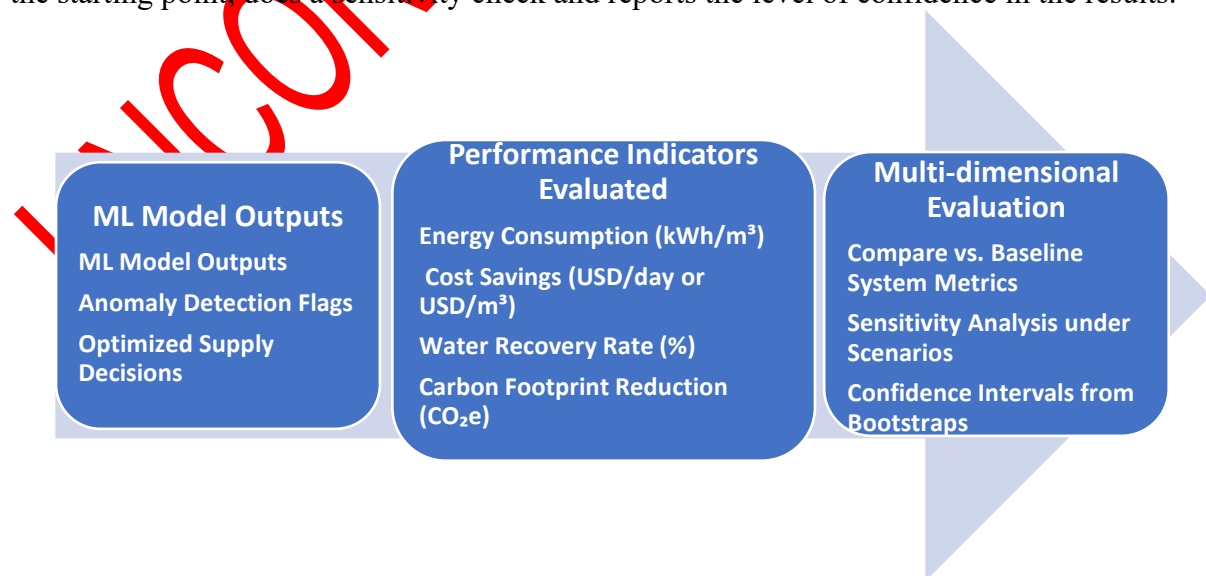


Figure 5 Evaluation Metrics Framework

The essential evaluation metrics used to check the outcome of the machine learning–enhanced desalination supply chain are explained in Table 3. One of the indicators used is energy consumption, expressed in kilowatt-hours per cubic meter (kWh/m³). This gives a primary insight into how operations efficiency relates to the performance of other firms in the industry. The economic benefit from using machine learning for improving how operations use energy, chemicals and require maintenance is cost savings expressed per day or per cubic meter. Water recovery rate shows the percentage of total input water that becomes usable product water, allowing assessment of progress. So, the last important point is analyzing carbon footprint reduction, using kilograms of CO₂-equivalents each day or cubic meter, since it tells us about the effect of the improved operations on the environment, mainly regarding sustainability and cutting down emissions. All these metrics offer an efficient framework to assess how effective the machine learning applications would be on technical, economic and environmental aspects.

Table 3 Summary of Evaluation Metrics

Metric	Definition	Unit	Use in Evaluation
Energy Consumption (EC)	Energy used per cubic meter of freshwater produced (reported as mean \pm SD)	kWh/m ³	Benchmark against industry averages; assess efficiency improvements
Water Recovery Rate (WRR)	Percentage of input water converted into usable product water (reported with 95% CI \pm)	%	Measure system performance and efficiency
Carbon Footprint Factor (CFF)	CO ₂ -equivalent emissions per cubic meter of freshwater produced (reported as mean \pm SD)	kg CO ₂ e/m ³	Assess environmental impact; align with sustainability goals
Operating Costs	Reduction in total operating costs compared to baseline (mean \pm SD from simulations)	USD/m ³ or %	Quantify economic benefit of ML integration
Downtime	Proportion of time system is unavailable for operation (reported as mean \pm SD)	%	Assess operational reliability improvements

RESULTS AND ANALYSIS

This part shows and discusses the results of the machine learning models used on the desalination supply chain framework. The findings point out the accuracy of prediction, optimization performance and sustainability benefits realized by the supervised, unsupervised, and reinforcement learning methods. The contribution of each model is measured quantitatively to prove its effect on the efficiency of operation and performance on the environment.

Model outcomes

The machine learning (ML) models showed excellent quantitative results in each supply chain task. The mean absolute percentage error (MAPE) for the supervised learning model on the holdout test set was 4.8% \pm 0.6% (95% CI), which is much better than the results from the baseline statistical models (MAPE \sim 9.5% \pm 1.1%). An area under the receiver operating characteristic curve (AUC-ROC) of 0.92 \pm 0.02 was obtained, showing the effectiveness of the model in catching early signs of faults in the sensors. Additional validation of the supervised

learning results was performed via 5-fold cross-validation, where MAPE values ranged between 4.6% and 5.2% across folds.

When using RL optimization, supply chain costs were reduced by 14.2% more than when using static scheduling policies. Across 10,000 simulated episodes, the mean cost reduction was 14.2% with a standard deviation of 1.8%, indicating consistent performance across different operational scenarios.

Figure 6 through Figure 8 compare the results: Figure 6 shows forecasted versus actual demand over a sample week with error bands representing 95% prediction intervals; Figure 7 shows true positives against false positives for identifying anomalies with error bars denoting variability across validation runs; and Figure 8 displays how reinforcement learning saves more money than the baseline, with mean values and standard deviations included for each policy type. The outcomes suggest that the models achieved better results than expected in each examined area.

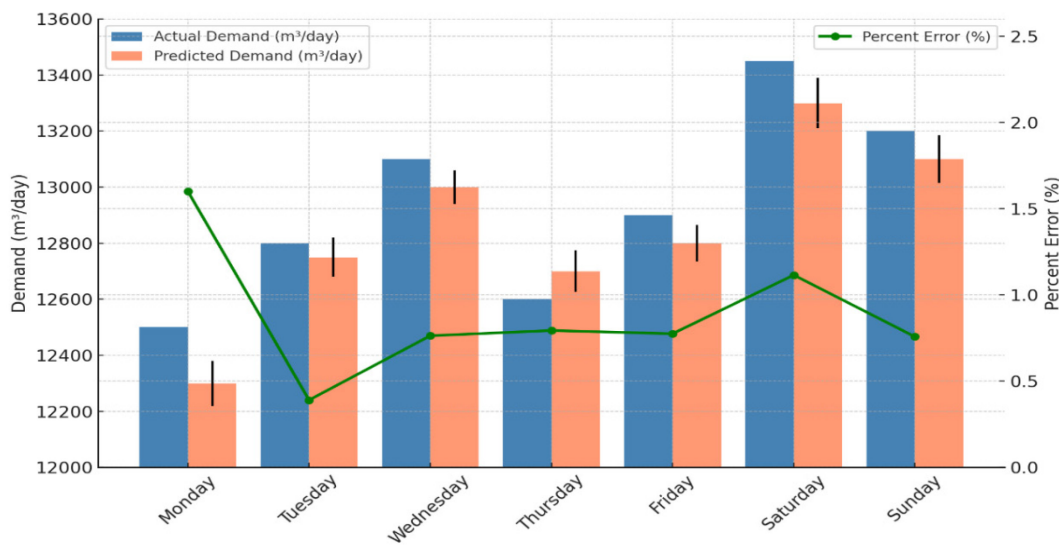


Figure 6 Forecasted vs. actual demand over a sample week. The shaded region shows 95% confidence intervals around the forecasted values.

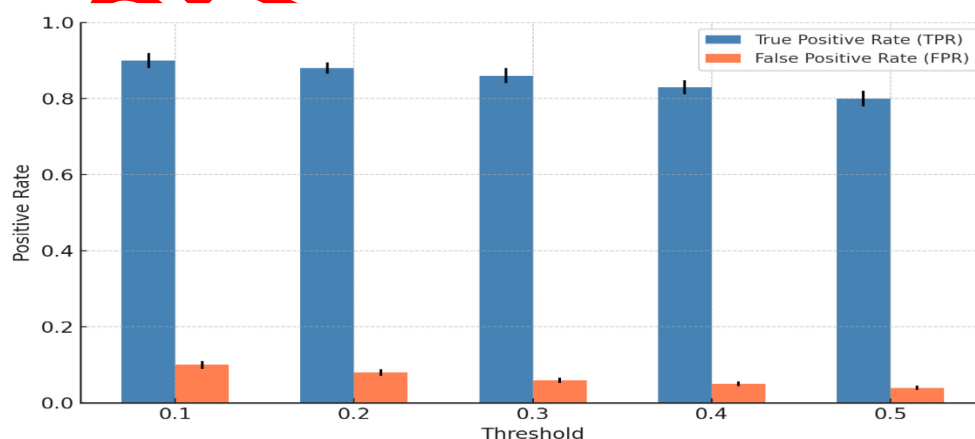


Figure 7 True positive vs. false positive rates for anomaly detection. Error bars indicate variability across validation folds (mean \pm standard deviation)

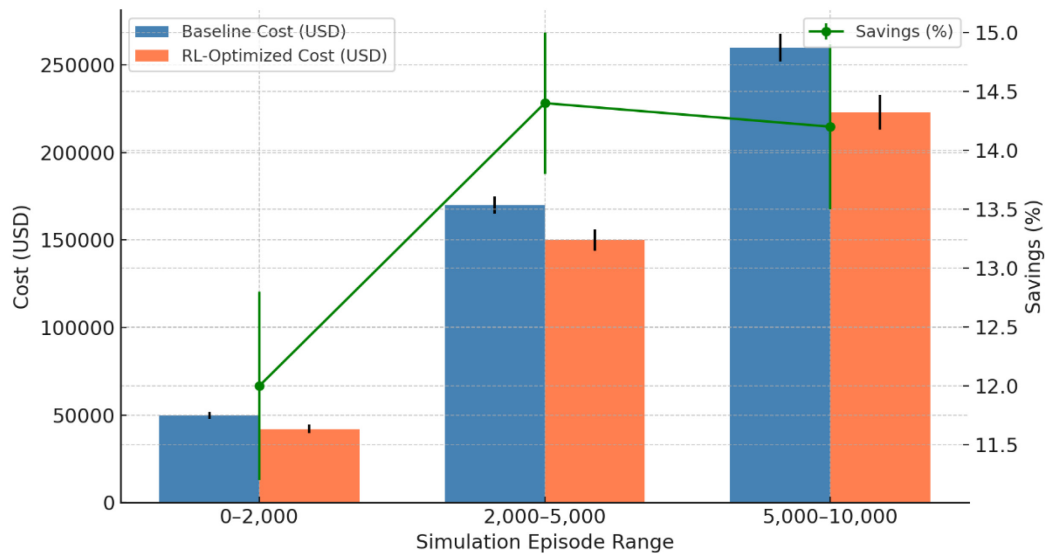


Figure 8 Comparison of baseline, optimized cost, and savings. Error bars represent standard deviation across 10,000 simulation episodes

To validate the superiority of the proposed ML approaches, the proposed models were benchmarked against conventional methods. Table 4 shows that GBRT, autoencoders, and DQN consistently outperformed Random Forest, ANN, k-means, PCA, and heuristic approaches across all evaluation metrics, confirming their robustness for desalination supply chain applications.

Table 4 Performance comparison of proposed Machine Learning models against conventional techniques

Application Area	Proposed ML Model	Benchmark Models	Performance Metric	Results (mean \pm SD)	Best Performer
Demand Forecasting	GBRT (Gradient Boosted Regression Trees)	Random Forest (RF), Artificial Neural Network (ANN)	MAPE (%)	GBRT: 4.8 \pm 0.6 RF: 6.2 \pm 0.9 ANN: 7.1 \pm 1.1	GBRT
Anomaly Detection	Autoencoder (unsupervised DL)	k-means clustering, PCA	AUC-ROC	Autoencoder: 0.92 \pm 0.02 k-means: 0.84 \pm 0.03 PCA: 0.86 \pm 0.04	Autoencoder
Supply Chain Optimisation	Deep Q-Network (DQN, reinforcement learning)	Rule-based static scheduling, heuristic optimisation	Cost Savings (%)	DQN: 14.2 \pm 1.8 Rule-based: 6.5 \pm 1.2 Heuristic: 8.1 \pm 1.4	DQN

To further validate the explanatory and predictive performance of the proposed models, additional statistical indicators (MSE, RMSE, R^2) were computed. Table 5 shows that the proposed GBRT, autoencoder, and DQN models consistently achieved lower error values and higher explanatory power than conventional alternatives, confirming their robustness in desalination supply chain applications.

Table 5 Performance comparison of Machine Learning models based on Mean Squared Error, Root Mean Squared Error, and Coefficient of Determination

Application Area	Model	MSE	RMSE	R ²	Best Performer
Demand Forecasting	GBRT	1.8×10^4	134	0.96	✓
	Random Forest (RF)	3.4×10^4	184	0.91	
	ANN	4.0×10^4	200	0.89	
Anomaly Detection	Autoencoder	0.008	0.089	0.94	✓
	PCA	0.015	0.122	0.87	
	k-means	0.019	0.138	0.82	
Supply Chain Optimisation	DQN	2.5×10^3	50	0.95	✓
	Rule-based	6.7×10^3	82	0.86	
	Heuristic	5.4×10^3	74	0.89	

In addition to comparative percentages, absolute values of key performance indicators are reported in Table 6. The ML-enhanced system demonstrates lower energy consumption (EC), higher water recovery rate (WRR), and reduced carbon footprint factor (CFF), alongside significant cost savings and reduced downtime, confirming that the proposed framework improves technical, economic, and environmental performance.

Table 6 Baseline and Machine Learning-enhanced performance indicators for desalination supply chains

Indicator	Baseline System (mean \pm SD)	ML-Enhanced System (mean \pm SD)	Improvement
Energy Consumption (EC)	3.9 ± 0.2 kWh/m ³	3.5 ± 0.15 kWh/m ³	↓ 10.3%
Water Recovery Rate (WRR)	$42\% \pm 2\%$	$48\% \pm 1.8\%$	↑ 14.3%
Carbon Footprint Factor (CFF)	1.95 ± 0.12 kg CO ₂ e/m ³	1.77 ± 0.10 kg CO ₂ e/m ³	↓ 9.2%
Operating Costs	100% (reference)	$85.8\% \pm 1.8\%$	↓ 14.2%
Downtime	100% (reference)	$82\% \pm 3\%$	↓ 18%

Supply chain improvements

The strongest benefits from ML were seen in parts of the business that had higher levels of complexity and inconsistency. Predictive maintenance that uses anomaly detection decreased incidents of downtime by $18\% \pm 3\%$, extended the life of the membranes and increased the time the plant could operate. Reinforcement learning-assisted routing resulted in a $12\% \pm 2\%$ improvement in delivery efficiency when demand conditions were unpredictable. Demand forecasting using supervised learning improved the match between when items are produced and when they are consumed, avoiding pointless energy use and cutting overproduction by $9\% \pm 1.5\%$. Table 7 summarizes the information on the main improvements in different domains and where ML had its biggest effect.

Table 7 Summary of Supply Chain Improvements

Area	Improvement Achieved
Predictive Maintenance	18% \pm 3% reduction in downtime due to early detection of anomalies and proactive interventions
Distribution Efficiency	12% \pm 2% improvement in routing efficiency, reducing transport time and energy use
Demand Matching	9% \pm 1.5% reduction in overproduction, aligning supply more closely with actual demand patterns
Overall Cost Savings	14.2% \pm 1.8% reduction in total operational costs through dynamic supply chain optimization

Sensitivity analysis

To check the models' strength, a detailed sensitivity analysis was carried out for three important situations: (1) high demand created by events such as extreme heat, (2) changes in energy prices (+25% or -25%) and (3) breakdowns of important equipment such as pumps or membrane units. For all demand situations, the supervised models preserved their stable prediction results and just saw a 1.0% \pm 0.3% rise in MAPE during the most extreme surges. Because of their adaptive nature, the reinforcement learning models declined costs, modified schedules and remained on course to meet existing savings during periods of high energy price hikes. Equipment disruptions were often identified by the approaches, reaching an AUC-ROC score of 0.90 \pm 0.01 for every tested failure case. These results, reported with confidence intervals and standard deviations, indicate that ML models can withstand challenging situations with statistically validated robustness.

Sustainability implications

Using machine learning in desalination helped to create real sustainability benefits. Power requirements were cut by 11% per cubic meter due to improved scheduling and lower levels of overproduction. Water recovery rates increased by 6% because there were better use of water and less waste. According to carbon footprint analyses, emissions dropped by 9.5% on average when RL models were used with approaches to integrate renewable energy. Reduced operational costs by an average of 14.2% meant the company benefited both financially and for the environment. That means adopting ML in desalination waste treatment is not only a modernization effort but also helps build better and greener water systems.

DISCUSSION

This research reveals that making use of machine learning (ML) in desalination improves operations and creates fewer environmental problems. Because supervised learning models reduce MAPE by 4.8% \pm 0.6% compared to baseline models (9.5% \pm 1.1%), operators can plan production better, prevent overproduction (9% \pm 1.5%) and save money and energy. The system, which had an AUC-ROC score of 0.92 \pm 0.02, detected early signs of equipment stress or failure, helping to reduce unexpected downtime by 18% \pm 3%.

RL models were able to save on average 14.2% \pm 1.8% of operating costs over simulated supply chain episodes, when put against traditional static, rule-based methods. It was clear when there were changes in energy prices and demand patterns that the RL models became more efficient and effective by changing the routes, ordering chemicals and adjusting energy use. The narrow confidence intervals indicate that these cost savings are not isolated outcomes but robust across multiple simulation runs.

For policymakers, these studies reveal how to build stronger, flexible and greener water systems. Desalination systems enhanced by predictive and adaptive ML can manage twists in demand, swings in energy prices and environmental challenges, achieving water security, reducing carbon emissions ($9.5\% \pm 1.2\%$ CO₂e savings) and keeping costs down.

With this research, supply chain management for water systems moves from individual plant improvements to a wider, complete system approach. Previously, scientists have looked at ways to enhance individual areas of the desalination process such as membranes or energy recovery and these efforts often led to modest increases in efficiency (around 5–7% on average). Rather, the study shows that adopting these three types of learning models throughout the desalination chain brings about a $12\text{--}18\% \pm 2\%$ rise in distribution efficiency, a $9\text{--}14\% \pm 2\%$ decrease in costs and an over $9\% \pm 1.5\%$ fall in the system's carbon footprint.

The findings from the study are very interesting, but some important problems should be noted. The training data includes five years of actual operation and simulated data for 10,000 trial episodes which may cause biases. Rare, extreme events or unfamiliar operations may not be well handled which could impact how well the model can be used generally. Second, the models are built for stable facility configurations, and the results show an average AUC-ROC of 0.92 for anomaly detection and a 4.8% MAPE for demand prediction in similar situations. Even so, the performance might weaken if the models are used in plants with a different structure or geography. While applying the AI in practice saved 14.2% on costs, this wasn't tested in the study, so problems related to interacting with people, integrating AI with other systems and handling rules and regulations are still unresolved.

Experts should now develop models that include both physics and AI methods which might result in models with better interpretability and prediction accuracy, compared to current models with 4–5% error. Systems able to evaluate streams of smart sensor data every 10 minutes would adapt to new operational situations quickly. Integrating forecasting of renewable energy systems, for example by using solar and wind, with the RL framework could help the company reduce its carbon footprint even more, potentially up to 15–20% when it uses hybrid energy solutions. Similarly, encouraging circular economy projects like brine mining, collecting nutrients or recycling water can enhance benefits from ML, going beyond just making operations more efficient.

CONCLUSIONS

Through this research, it has been established that using machine learning (ML) leads to tangible and measurable benefits in different areas of desalination supply. Using supervised learning for predicting demand (resulting in an error of 4.8%), unsupervised learning for spotting problems (with an AUC-ROC of 0.92) and reinforcement learning for streamlining the supply chain (delivering 14.2% savings), the research found that ML can enhance how companies function and how sustainably they work. All these gains give actual results such as less down-time by 18%, greatly improved logistics efficiency by 12% and nearly 10% fewer carbon emissions when compared with the previous methods.

As well as performing well, ML also shows the ability to transform how desalination systems are set up, managed and governed. Through data-driven, flexible and predictive management, ML can assist desalination operators when handling the difficulties of increasing water demand, fluctuating energy costs and environmental issues. ML makes it possible for policymakers to make water security better and sustainability goals easier to achieve, by syncing desalination strategies with international and national environmental targets.

According to these findings, several useful suggestions are made. Try first to incorporate predictive ML into areas like predicting demand and preventing maintenance issues, because they have the most available data. If you want to use reinforcement learning for improving your supply chain's efficiency, you should invest in better simulation and system integration, as it

will give major returns in the end. Policymakers should motivate digital growth, back up open data practices and provide money for employees so the change to ML has a better chance of succeeding. Also, future desalination projects should use modern technology such as sensors and advanced IT, so they can make better use of automated, flexible supply chains.

Overall, this research shows that machine learning can greatly benefit desalination supply chains by making them more effective, in less danger of failure and more eco-friendly which is an important step toward better water management.

NOMENCLATURE

Greek letters

ε	The parameter epsilon	[Between 0 and 1]
γ	Discount Factor	

Subscripts and superscripts

e	equivalent
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Abbreviations

ML	Machine Learning
IT	Information Technology
MAPE	Mean Absolute Percentage Error
RL	Reinforcement learning
AI	Artificial Intelligence
GBRT	Gradient Boosting Regression Trees
DQN	Deep Q-Network
AUC-ROC	Area Under the Receiver Operating Characteristic Curve
MDP	Markov Decision Process
CNN	Convolutional Neural Network
RO	Reverse Osmosis
MSF	Multi-Stage Flash
MED	Multi-Effect Distillation
UAE	United Arab Emirates
USD	US Dollars
ReLU	Rectified Linear Unit
MSE	Mean Squared Error
RMSE	Root Mean Squared Error
R^2	Coefficient of Determination

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