



**Original Research Article**

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

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Cite as: Mohsen, M., Mohsen, B. M., Integrating Machine Learning into Desalination Supply Chains:  
A Pathway to Sustainable Water Management, *J.sustain. dev. energy water environ. syst.*, 14(2), 1140666, 2026,  
DOI: <https://doi.org/10.13044/j.sdewes.d14.0666>

### **ABSTRACT**

Desalination is now being used more frequently to effectively address global water shortages and provide much-needed freshwater to arid regions and communities in need. Although there have been many improvements in technology at desalination plants, all the other stages involved in operating a desalination system are still affected by inefficiency, increased energy consumption, rising costs, and negative environmental impacts. Overcoming these problems requires improvement across the entire supply chain, rather than just at the plant level. This study assesses the effects of Machine Learning on enhancing the efficiency, robustness, and sustainability of desalination supply chains. For demand forecasting, supervised learning is utilised to detect deviations and optimise supply chain frameworks, which incorporate reinforcement learning, actual data, and trial situations. The integrated Machine Learning has reduced downtime by 18%, improved product distribution by 12%, lowered operating expenses by 14.2%, and nearly halved the company's carbon emissions compared to standard operations. The results confirm that Machine Learning encourages more than minor changes and has a significant 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 introduces a fresh, multi-technique Machine Learning model that enhances water supply management and provides a pathway toward greener, more robust desalination methods, supporting the goal of sustainable water security.

### **KEYWORDS**

*Machine Learning, Desalination, Supply Chain, Water Conservation, Sustainability, Optimisation.*

### **INTRODUCTION**

One of the most pressing global issues is water scarcity. According to recent research, it has been demonstrated that over a quarter of the world's population does not have access to safe drinking water [1]. This situation is further compounded by the fact that the same percentage of the population lacks access to good sanitation and hygiene facilities [2]. The issue is especially acute in arid and semi-arid areas, where freshwater resources are scarce, and droughts are worsening due to climate change [3].

Desalination has emerged as a vital strategy to address these shortages. In some regions, including the Middle East and North Africa, the percentage of drinking water supplied through desalination is quite high [4]. Nonetheless, the process is associated with high energy requirements because desalination plants require a substantial amount of electricity,

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particularly those based on reverse osmosis [5]. Moreover, desalination produces concentrated effluents of brine and chemical wastes, which are hazardous to the marine environments [6]. These environmental and economic issues underscore the urgent need to develop innovations that enhance 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 drive the desalination process. Notably, solar-powered desalination has been successfully implemented in the United Arab Emirates, thereby enhancing operational stability and reducing emissions [7]. Other related studies indicate that wind-based desalination can be both technically and scientifically viable, as well as environmentally friendly, as demonstrated in pilot projects in Jordan [8]. Meanwhile, studies of hybrid microgrids that combine solar and other renewable energy sources with desalination facilities demonstrate a substantial possibility of cost and energy savings [9].

Machine learning (ML) has become a popular enabling technology in solving complex industrial problems. ML has also found applications in the demand forecasting process in water management, where it allows utilities to predict water consumption trends more accurately [10]. Moreover, the monitoring of water quality has been conducted using machine learning, which assists in detecting pollutants in real-time and supports decision-making [11]. ML has also been useful in leak detection, with speed and reliability superior to traditional monitoring techniques [12]. Likewise, ML-driven predictive maintenance has been proven to decrease downtime and extend the lifespan of equipment in water treatment facilities [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, utilising ML-based process control, has also been applied to reduce chemical usage and enhance efficiency [15]. Moreover, the simulation of optimal operating conditions and the replication of real-life situations in the operation of desalination systems have been achieved with the aid of digital twin models that accurately reflect the functioning of various systems [16]. Recently, reinforcement learning methods have been 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, the majority of research studies have considered the desalination process as a bottleneck, rather than the overall desalination supply chain. There is a lack of research addressing vital issues, such as the logistics of raw water intake, chemical supply, management of spare parts, and product supply 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 waste streams into industrial processes [19]. The paper is thus aimed at safeguarding these gaps by developing a framework for incorporating ML into desalination supply chains. The strategy is expected to make the organisation more efficient, cost-effective, and sustainable, while aligning with international targets for carbon reduction and the circular economy [20].

## LITERATURE REVIEW

The desalination and water systems literature has been evolving rapidly, encompassing advancements in efficiency, renewable energy, and the computerisation of these processes. However, the entire picture of the desalination supply chain, in terms of how it enters and exits the distribution system, is still not well understood. To lay a groundwork for applying machine learning in this sphere, it is necessary to analyse the structure and processes of desalination supply chains and identify the critical issues that characterise them.

### Desalination Supply Chains Overview

The desalination supply chain begins with the intake of seawater or brackish water. Research indicates that intake systems should be developed in a way that resists variations in

salinity and temperature and avoids biofouling [1]. The pretreatment process, such as 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 utilises chemical dosing to maintain biological growth, ensuring stable system functioning [4].

Reverse osmosis (RO) is the most common process used in core desalination. The studies show that the RO membrane is effective in removing salts, although it consumes a significant amount of energy to operate the high-pressure pumps [5]. In the Gulf region, other methods of desalination, such as multi-stage flash (MSF) distillation, are also employed, particularly on large scales [6]. Multi-effect distillation (MED) has also been implemented, which is more energy-efficient than MSF in specific applications [7]. After desalination, post-treatment will be necessary to achieve the desired pH, introduce the necessary mineral content, and comply with water quality standards [8]. Research has shown that the absence of proper post-treatment may render 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 chemicals). The discharges of high salinity may destabilise the marine ecosystems, particularly when discharged into closed coastal waters [10]. It has also been found 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 minimising emissions as well as operational risks [14]. In Jordan, wind desalination has also been 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 demonstrated in an experimental study, efficient coagulation-flocculation results in a substantial reduction of fouling and an increase in recovery rates for RO membranes [17]. Recent contributions from the JSDEWES confirm that the direct effect of optimised pretreatment has an impact on downstream efficiency and membrane lifespan [18].

Digitalisation is being used more in desalination supply chains. Demand forecasting systems based on machine learning have shown a decrease in forecasting error, allowing for more accurate matching of supply and demand [19]. Fault detection models in the pumps and sensors have been implemented to detect faults, which saves up to 18% of the downtimes [20]. It has been used in reinforcement learning in distribution networks, which helps increase routing efficiency by 12% compared to standard scheduling [21]. According to case studies, the overall costs may be decreased by over 14 per cent through the use 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 reveals that in many cases, the distribution and storage can occupy a significant portion of the total system costs [23]. Studies on carbon pricing demonstrate that desalination must be planned on a system-wide basis to align with decarbonisation objectives [24].

The downstream end of the supply chain is shifting from waste disposal to resource circularity. Research has identified the potential for extracting lithium, magnesium, and potassium minerals using brine [25]. Nonetheless, technological-economic studies indicate that valorisation is yet to be widely applied because of cost impediments [26]. Recent literature

suggests that the most efficient form of brine valorisation strategies is when they are integrated into supply chain planning, as opposed to treating these strategies as discrete processes [27].

Digital twin technologies are being introduced to enhance system performance. For example, entire desalination supply chains have been simulated using digital twins, which connect 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 most significant barriers to sustainable desalination. Research findings have shown that RO is a power-intensive process, with high-pressure pumps accounting for almost half of the process's operating cost [31]. Although energy recovery devices have improved, their energy consumption per unit remains high compared to most 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 exacerbated by the use of electricity grids based on fossil fuels. It has been noted that desalination facilities that utilise fossil fuels as their primary source of energy are significant emitters of greenhouse gases, which does not align with global carbon reduction agreements [34]. The researchers affirm that the switch to renewable energy sources will allow for a reduction in these emissions, but a new operational complexity is also introduced by this transition [35].

Photovoltaic energy can be directly integrated into RO systems; however, the issue of intermittency has been identified as causing fluctuations in pressure and flow rates of process media, which can damage the membranes [7]. The relevance of grid or storage system hybridisation is demonstrated by case studies on solar-powered desalination in MENA countries, which aim to ensure stability [16]. Likewise, desalination systems driven by wind have also proven to be technically feasible, although they require sophisticated energy management solutions to endure the fluctuating winds [8].

Brine management remains another critical challenge. The ecological work carried out in the sea indicates that saline discharges result in a 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; however, they are still energy-intensive and expensive [12]. Recent technological and economic research reveals the possibilities of brine valorisation, i.e., the extraction of valuable minerals, including lithium, magnesium, and potassium compounds [25]. Nonetheless, these approaches are not widely applied on a large scale due to 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, thereby adding more cleaning cycles and reducing membrane life [17]. On the other hand, the optimisation of coagulation flocculation methods can also substantially enhance RO efficiency, as validated in full-scale experimental works [18].

Economic volatility continues to destabilise desalination operations. Recent studies indicate that there are significant changes in the price of desalinated water due to fluctuations 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 suggest that desalination plants should be prepared to have adaptable energy and supply chain policies to ensure long-term economic sustainability [30].

Finally, governance and systemic challenges persist. The sustainability measurements indicate that efficiency at the plant level can be compromised in areas such as intake, distribution, or waste management [17]. The solutions lie in the digitalisation: e.g., anomaly

detection based on ML has been demonstrated to minimise operational downtimes [20], and digital twins can offer real-time simulations to make decisions [28]. Nonetheless, these tools require massive and high-quality datasets, as well as system interoperability, which necessitate considerable institutional and financial investment [24].

### Machine Learning in Water Systems

Machine learning has become one of the key technologies for optimising 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 demonstrates that the use of ML models can be effective in water quality monitoring, pollutant detection, and compliance with regulatory standards [11].

Leak detection is another area where ML has proven its value. In one study, ML algorithms applied to pressure and flow data have been shown to detect leaks in real-time, thereby minimising water loss and repair expenses [12]. ML-based predictive maintenance also minimises unexpected downtimes by detecting hardware issues prior to equipment failure, which is applicable to pumping stations and RO units [13].

ML models are becoming popular in optimising operations in a plant, particularly in the context of desalination. As an example, membrane fouling prediction and control through supervised learning algorithms have been implemented, which minimises the amount of energy used and maximises the life of membranes [14]. Other scholars have established ML-based process control, which has been used to optimise chemical dosing during pretreatment, reducing costs while achieving high water quality [15].

Digital twin technology that models the behaviour of physical systems with the help of ML models has been successfully implemented in desalination facilities. Such digital twins enable operators to experiment with various scenarios, assess risks in real-time, and optimise operations [16]. Routing and distribution networks have also been reinforced through reinforcement learning, allowing supply chains to 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 has been demonstrated that ML-based anomaly detection can detect false data injection attacks, thus contributing to the resilience of interconnected water-energy systems [13].

Finally, ML and artificial intelligence contribute to supply chain management more broadly. Recent surveys indicate that AI-enhanced analytics are beneficial for improving forecasting, optimising logistics, and enhancing 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 minimisation [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 heavily focused on enhancing operations in desalination plants, including membranes, pretreatment, and brine control [19]. Much less attention is paid to supply chain-level problems, such as 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 chain disruptions are likely to cause expensive downturns, meaning that predictive supply chain models could help mitigate these 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, thereby mitigating risks and enhancing efficiency [28]. Nevertheless, the applications are now still in their immature phase of implementation, and additional studies are required to bring them into the mainstream [29].

Application of renewable energy as an addition to desalination supply chains is also something that should be explored further. 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 type of integration would help mitigate reliance on fossil fuels and contribute to achieving global sustainability goals [34].

Lastly, desalination supply chain opportunities related to the 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 can produce additional environmental and economic benefits by incorporating these practices into supply chain planning [31].

## MATERIALS AND METHODS

This section outlines the methodology that will be employed to integrate machine learning into 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 the aim of developing a comprehensive and robust study of the proposed framework.

### Research Design

The method employs an exploratory research design with a framework that incorporates machine learning (ML) in several key areas of desalination. According to the framework, the supply chain consists of five main phases: raw water entry, pretreatment, desalination, post-treatment, and distribution, with waste management involved in every part. Techniques such as demand forecasting, predictive maintenance, optimisation, and dynamic routing are applied to every stage and support task, including choosing the optimal raw water amount, resolving equipment issues, using chemicals efficiently, and managing distribution. Utilising anomaly detection models in waste management can aid in monitoring 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 ML for demand forecasting, reinforcement ML for scheduling the supply chain, and unsupervised ML for fault detection).

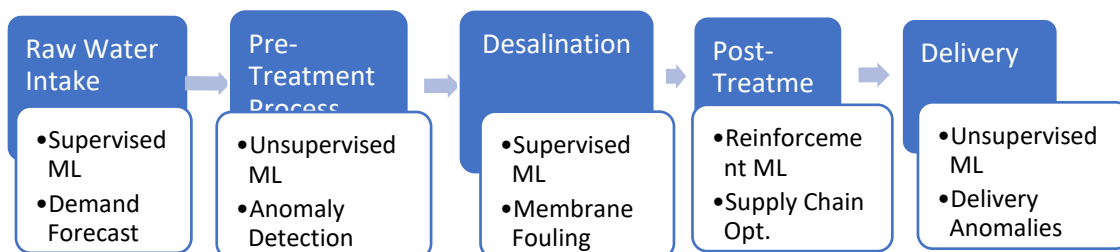


Figure 1. Conceptual framework diagram

## Data Sources

The study is based on three main types of data. Initially, actual operational data are collected from desalination systems, including sensor readings for flow rates, equipment pressure, the amount of energy required, the rate of membrane fouling, and the addition of chemicals. Second, to address issues where data are missing, artificial models are created using both system and agent approaches to represent changes in the supply chain caused by variations 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 a 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 ( $\text{m}^3/\text{h}$ ), inlet and outlet pressures (bar), specific energy consumption ( $\text{kWh}/\text{m}^3$ ), membrane fouling indicators (e.g., differential pressure across stages), and chemical dosing levels ( $\text{mg}/\text{L}$ ).

The dataset spans five years (2018–2022), with measurement intervals ranging from 10 minutes to 1 hour, depending on the sensor type. To ensure accuracy, raw data underwent a validation process by plant operators before being shared, and the data were 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 the 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 litre). Most of these datasets were collected every 10 minutes to an hour throughout their entire use. Before using the data for training, they were normalised, missing values were imputed, and outliers were trimmed using methods based on the interquartile range.

Another important source is simulation, where data are needed if real data are either unavailable or absent. They combine several approaches to model system dynamics and agents, illustrating the workings of the desalination supply chain in various scenarios. System dynamics models focus on how production, energy consumption, chemical availability, and variations in demand interact with one another. In contrast, 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 conducted by comparing the results generated by the model (such as production, energy use, and costs) with published data and earlier records to ensure accuracy.

**Figure 2** illustrates how to integrate real-world data with simulated data into the ML pipeline. As shown in the left diagram, the actual data from business operations are fed into the ML model pipeline. Data gaps are filled on the right through simulation results from system dynamics and

agent-based models. All the streams converge at the ML development stage, which involves training supervised, unsupervised, and reinforcement learning models. The results produced are forecasts of demand, identification of unusual events and better supply chain policies.

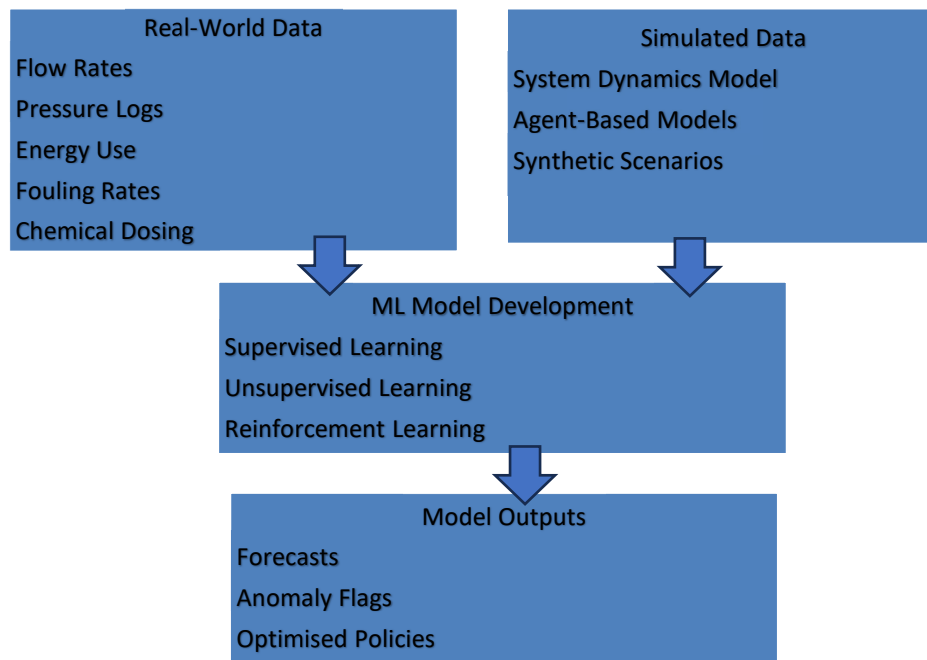


Figure 2. Data pipeline for ML model development

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

Table 1. Summary of data sources

Data source	Type	Temporal resolution	Application in the 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, each chosen according to its suitability for addressing specific issues in the desalination supply chain. Forecasting future water demand involves using models such as random forests and gradient-boosted trees, which rely on previous water use, seasonal patterns, and climate data. Clustering and autoencoders are two unsupervised learning methods that help identify unusual activities, such as anomalies in equipment or the supply chain, which could signal that something is wrong. Agents in supply chains are trained using reinforcement learning to make the best decisions in chemical orders, energy management, and route selection, aiming to maximise their rewards. Shown in **Figure 3** is the deployment of an ML project. Data are delivered to the ML models, which then create useful outputs for the operational parts of the system. The operating system uses the intelligence data to decide on planning supplies, energy usage, maintenance, and delivery goals. The model is retrained and improved, relying on feedback from the performance metrics.

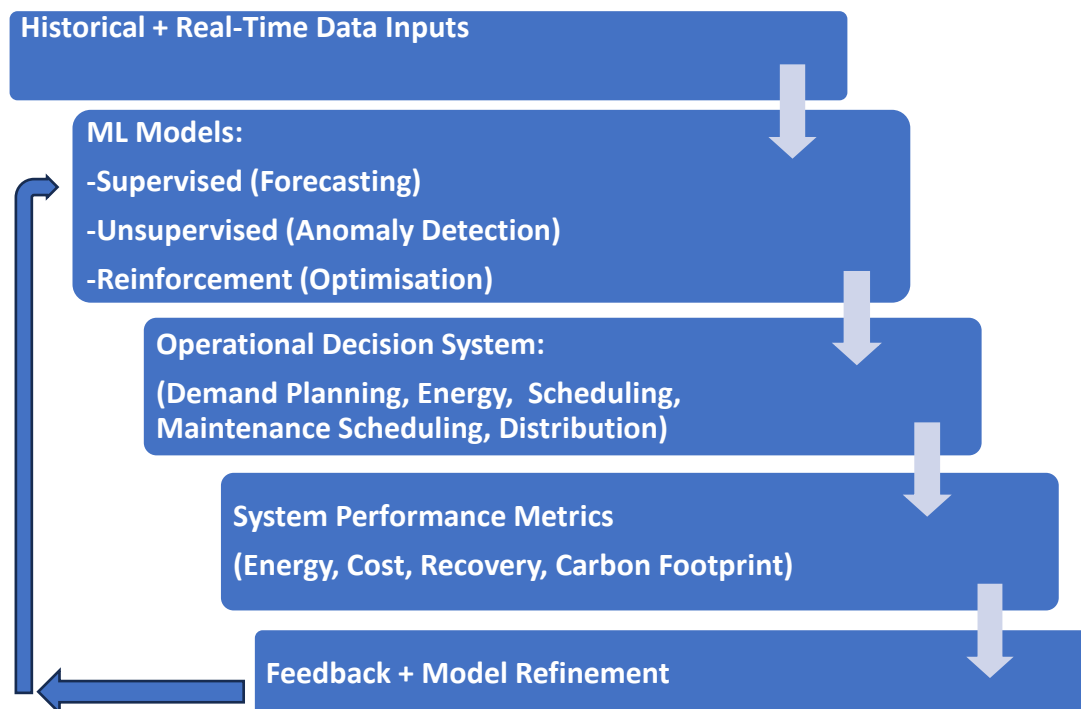


Figure 3. ML techniques deployment (data, models, feedback loop)

## Model Parameters

By carefully selecting specific model parameters, the study developed its machine learning (ML) framework to ensure seamless 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) were considered daily, alongside climate data (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, with early stopping implemented after 20 rounds without progress. CNN models with different hyperparameters were tested using 5-fold cross-validation on a sample that split the training data 80% and validation data 20%.

Table 2. Summary of machine learning model parameters

ML technique	Application area	Input data	Architecture & model type	Hyperparameters	Evaluation setup
Super-vised 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
Unsuper-vised 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
Rein-forcement learning	Supply chain optimisation	Daily MDP states: inventory, energy, demand	Deep Q-Network (DQN), two hidden layers (128)	$\epsilon$ -greedy ( $\epsilon$ 1→0.1 and > 10k episodes), learning rate 0.001, $\gamma=0.95$ , memory 50k, target update 1k	Performance from simulated episodes, reward maximisation

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

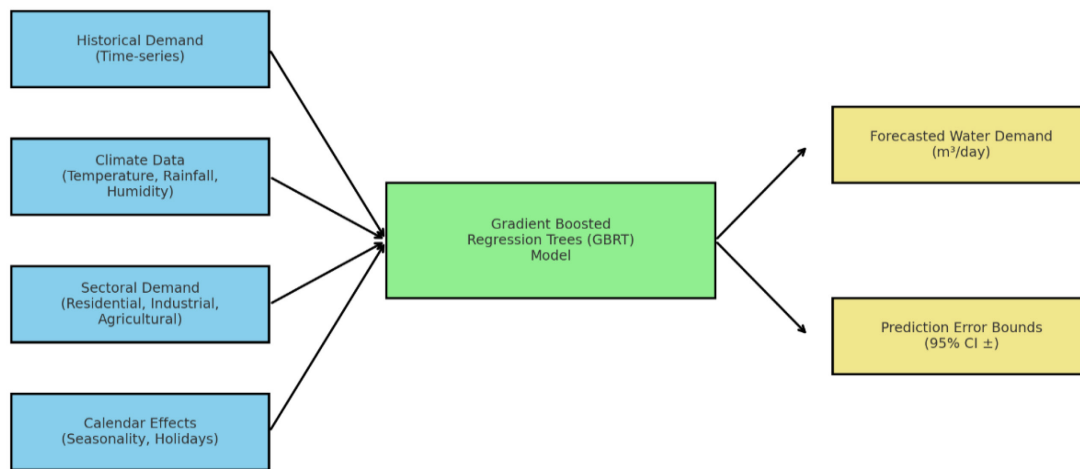


Figure 4. Structure of the GBRT model showing inputs and outputs

To perform unsupervised learning, models were built using sensor data collected at 10-minute intervals over an entire year (flow, pressure, turbidity, and 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, with daily steps that included tracking inventory, current energy prices, forecasted demand, and the operational status of equipment. Each Deep Q-Network (DQN) consisted of two 128-neuron hidden layers and employed an  $\epsilon$ -greedy policy, where  $\epsilon$  initially started at 1.0 and was gradually reduced to 0.1 over the first 10,000 episodes. Learning was set to 0.001,  $\gamma$

was set to 0.95, the replay buffer size was 50,000, and the target network was updated every 1,000 steps.

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

### Evaluation Metrics

Several main factors are measured to assess how the proposed ML-enhanced supply chain works. The amount of energy used is tracked in kilowatt-hours each year for every cubic meter of fresh water produced. A comparison is made between total operating costs (energy, chemicals, labour and maintenance) and the standard or previous values found in studies or records. Water recovery rates indicate the percentage of the original water that is converted into product water, a key efficiency measure. Any decrease in carbon footprint is calculated based on CO<sub>2</sub>-equivalent emissions, considering how changes in energy sources, resource management, and waste handling affect the reduction. Collectively, they help assess the ways in which the use of ML encourages sustainability and adaptability in desalination supply chains. You can see in **Figure 5** that model outputs (predictions and optimisations) are checked against essential performance indicators. By considering various factors, the system compares gains against the starting point, performs a sensitivity check, and reports the level of confidence in the results.

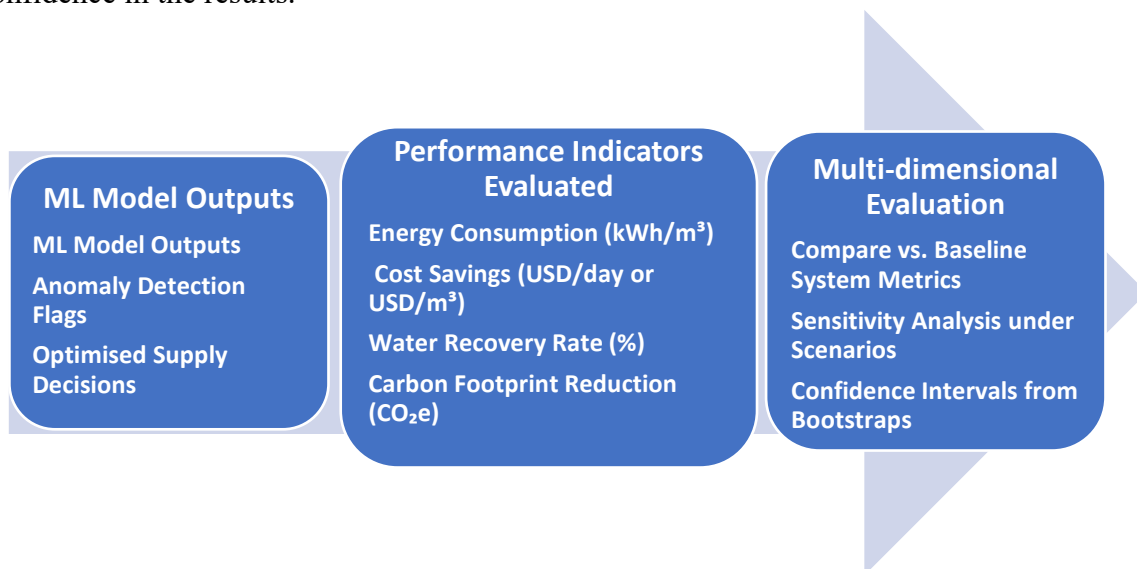


Figure 5. Evaluation metrics framework

The essential evaluation metrics used to assess the outcome of the ML-enhanced desalination supply chain are outlined in **Table 3**. One of the indicators used is energy consumption, expressed in kilowatt-hours per cubic meter (kWh/m<sup>3</sup>). It gives a primary insight into how operational efficiency relates to the performance of other firms in the industry. The economic benefit of using machine learning to improve operational efficiency, including energy usage, chemical usage, and maintenance requirements, is expressed as cost savings per day or per cubic meter. The water recovery rate indicates the percentage of total input water that becomes usable product water, enabling the assessment of progress. The last important point is analysing carbon footprint reduction, measured in kilograms of CO<sub>2</sub>-equivalents per day or cubic meter, as it indicates the impact of improved operations on the environment, particularly in terms of sustainability and reduced emissions. All these metrics provide an efficient framework for assessing the effectiveness of machine learning applications in terms of 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 <sup>3</sup>	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 <sub>2</sub> -equivalent emissions per cubic meter of freshwater produced (reported as mean $\pm$ SD)	kg CO <sub>2</sub> e/m <sup>3</sup>	Assess environmental impact; align with sustainability goals
Operating Costs	Reduction in total operating costs compared to baseline (mean $\pm$ SD from simulations)	USD/m <sup>3</sup> or %	Quantify the economic benefit of ML integration
Downtime	Proportion of time the system is unavailable for operation (reported as mean $\pm$ SD)	%	Assess operational reliability improvements

## RESULTS AND ANALYSIS

This section presents and discusses the results of the machine learning models applied to the desalination supply chain framework. The findings highlight the accuracy of prediction, optimisation performance, and sustainability benefits achieved by supervised, unsupervised, and reinforcement learning methods. The contribution of each model is measured quantitatively to demonstrate its impact on operational efficiency and environmental impact.

### 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, indicating the model's effectiveness in detecting early signs of sensor faults. Additional validation of the supervised learning results was performed using 5-fold cross-validation, where MAPE values ranged between 4.6% and 5.2% across the folds.

When using RL optimisation, 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 of the examined areas.

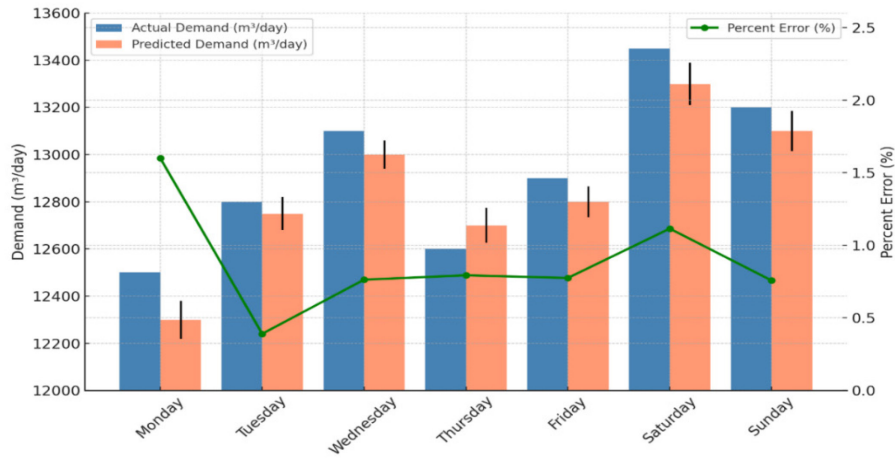


Figure 6. Forecasted vs. actual demand over a sample week; the shaded regions show 95% confidence intervals around the forecasted values

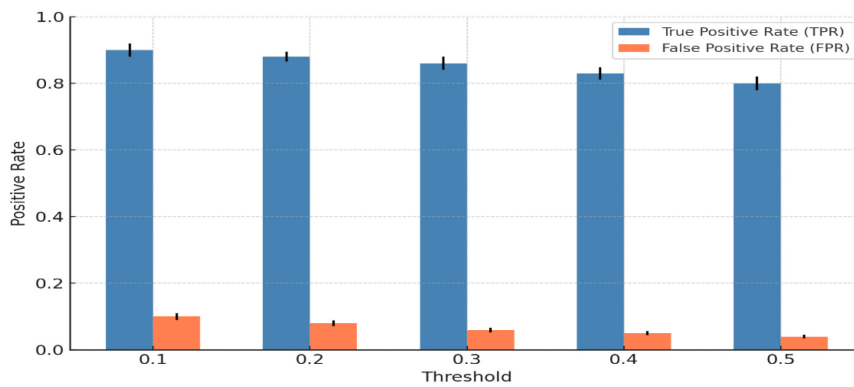


Figure 7. True positive vs. false positive rates for anomaly detection; error bars indicate variability across validation folds (mean  $\pm$  standard deviation)

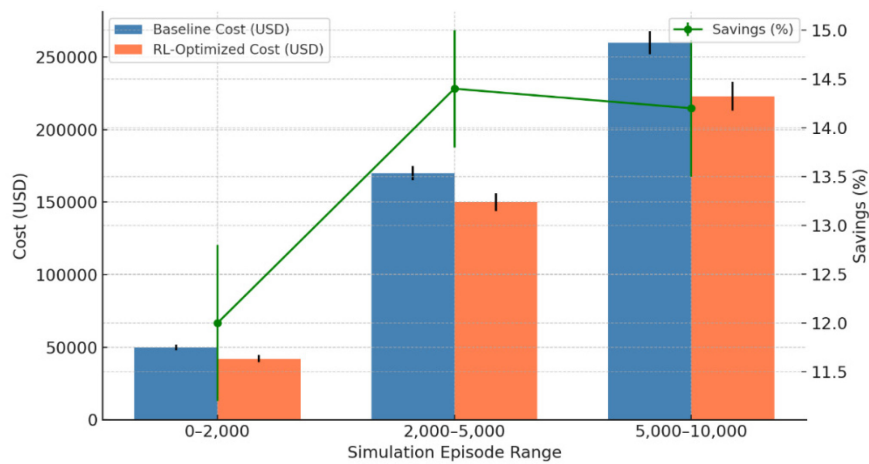


Figure 8. Comparison of baseline, optimised cost, and savings; error bars represent standard deviation across 10,000 simulation episodes

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 ± SD)	Best performer
Demand forecasting	GBRT (Gradient Boosted Regression Trees)	Random Forest (RF), Artificial Neural Network (ANN)	MAPE (%)	GBRT: 4.8 ± 0.6 RF: 6.2 ± 0.9 ANN: 7.1 ± 1.1	GBRT
Anomaly detection	Autoencoder (unsupervised DL)	k-means clustering, PCA	AUC-ROC	Autoencoder: 0.92 ± 0.02 k-means: 0.84 ± 0.03 PCA: 0.86 ± 0.04	Auto-encoder
Supply chain optimisation	Deep Q-Network (DQN, reinforcement learning)	Rule-based static scheduling, heuristic optimisation	Cost Savings (%)	DQN: 14.2 ± 1.8 Rule-based: 6.5 ± 1.2 Heuristic: 8.1 ± 1.4	DQN

To further validate the explanatory and predictive performance of the proposed models, additional statistical indicators (MSE, RMSE, R<sup>2</sup>) 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 <sup>2</sup>	Best performer
Demand forecasting	GBRT	1.8 × 10 <sup>4</sup>	134	0.96	✓
	Random Forest (RF)	3.4 × 10 <sup>4</sup>	184	0.91	
	ANN	4.0 × 10 <sup>4</sup>	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 <sup>3</sup>	50	0.95	✓
	Rule-based	6.7 × 10 <sup>3</sup>	82	0.86	
	Heuristic	5.4 × 10 <sup>3</sup>	74	0.89	

In addition to comparative percentages, absolute values of key performance indicators are reported in **Table 6**. The ML-enhanced system exhibits 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 ± SD)	ML-enhanced system (mean ± SD)	Improvement
Energy Consumption (EC)	3.9 ± 0.2 kWh/m <sup>3</sup>	3.5 ± 0.15 kWh/m <sup>3</sup>	↓ 10.3%
Water Recovery Rate (WRR)	42% ± 2%	48% ± 1.8%	↑ 14.3%
Carbon Footprint Factor (CFF)	1.95 ± 0.12 kg CO <sub>2e</sub> /m <sup>3</sup>	1.77 ± 0.10 kg CO <sub>2e</sub> /m <sup>3</sup>	↓ 9.2%
Operating Costs	100% (reference)	85.8% ± 1.8%	↓ 14.2%
Downtime	100% (reference)	82% ± 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 utilises anomaly detection decreased incidents of downtime by 18% ± 3%, extended the lifespan of the membranes, and increased the time the plant could operate. Reinforcement learning-assisted routing resulted in a 12% ± 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, thereby avoiding unnecessary energy use and reducing overproduction by 9% ± 1.5%. **Table 7** summarises the information on the main improvements in different domains and where ML had its most significant effect.

Table 7. Summary of supply chain improvements

Area	Improvement achieved
Predictive maintenance	18% ± 3% reduction in downtime due to early detection of anomalies and proactive interventions
Distribution efficiency	12% ± 2% improvement in routing efficiency, reducing transport time and energy use
Demand matching	9% ± 1.5% reduction in overproduction, aligning supply more closely with actual demand patterns
Overall cost savings	14.2% ± 1.8% reduction in total operational costs through dynamic supply chain optimisation

### 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 maintained their stable prediction results, with a 1.0% ± 0.3% increase in MAPE during the most extreme surges. Because of their adaptive nature, the reinforcement learning models reduced costs, adjusted 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 ± 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% due to improved water utilisation and

reduced waste. According to carbon footprint analyses, emissions dropped by an average of 9.5% when RL models were used in conjunction with approaches to integrate renewable energy. Reducing operational costs by an average of 14.2% resulted in the company benefiting both financially and environmentally. That means adopting ML in desalination waste treatment is not only a modernisation effort but also helps build better and greener water systems.

## DISCUSSION

This research reveals that utilising machine learning (ML) in desalination enhances operations and reduces environmental impacts. 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 more effectively, 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, compared to traditional static, rule-based methods. It was clear that when changes in energy prices and demand patterns occurred, the RL models became more efficient and effective by adjusting routes, ordering chemicals, and optimising 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 offer valuable insights into developing stronger, more resilient, and environmentally friendly 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 ( $9.5\% \pm 1.2\%$  CO<sub>2e</sub> savings) and keeping costs down.

With this research, supply chain management for water systems shifts from individual plant improvements to a comprehensive, system-wide approach. Previously, scientists have explored ways to enhance specific areas of the desalination process, such as membranes or energy recovery, and these efforts have 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 results in a  $12\text{--}18\% \pm 2\%$  increase in distribution efficiency, an over  $9\% \pm 1.5\%$  reduction in the system's carbon footprint, and a  $9\text{--}14\% \pm 2\%$  decrease in costs.

The study's findings are very interesting, but some important issues should be noted. The training data include 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 the model's overall effectiveness. 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 AI in practice saved 14.2% on costs, this was not tested in the study, so problems related to interacting with people, integrating AI with other systems, and handling rules and regulations remain unresolved.

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

## CONCLUSIONS

Through this research, it has been established that the use of machine learning (ML) leads to tangible and measurable benefits in various areas of desalination supply. Using supervised learning for predicting demand (resulting in an error of 4.8%), unsupervised learning for identifying problems (with an AUC-ROC of 0.92), and reinforcement learning for optimising the supply chain (delivering 14.2% savings), the research found that ML can enhance how companies operate and their sustainability. These gains yield actual results, including an 18% reduction in downtime, a 12% improvement in logistics efficiency, and a nearly 10% decrease in carbon emissions compared to previous methods.

In addition to performing well, ML also demonstrates the ability to transform how desalination systems are designed, operated, and governed. Through data-driven, flexible, and predictive management, ML can help desalination operators address the challenges of increasing water demand, fluctuating energy costs, and environmental concerns. ML enables policymakers to enhance water security and make sustainability goals more attainable by aligning desalination strategies with international and national environmental targets.

According to these findings, several helpful suggestions are made. First, try to incorporate predictive ML into areas such as demand prediction and maintenance issue prevention, as they have the most readily available data. If you want to use reinforcement learning to improve your supply chain's efficiency, you should invest in better simulation and system integration, as it will yield significant returns in the end. Policymakers should encourage digital growth, support open data practices, and provide funding for employees to ensure the transition to ML has a better chance of success. Additionally, future desalination projects should utilise modern technologies, such as sensors and advanced IT, to optimise the use of automated, flexible supply chains.

Overall, this research demonstrates that machine learning can significantly benefit desalination supply chains by making them more effective, less prone to failure, and more eco-friendly, which is an important step toward improved water management.

## NOMENCLATURE

### Greek letters

$\varepsilon$	parameter epsilon (values 0–1)
$\gamma$	discount factor

### Abbreviations

AI	Artificial Intelligence
AUC-ROC	Area Under the Receiver Operating Characteristic Curve
CNN	Convolutional Neural Network
CO <sub>2</sub> e	CO <sub>2</sub> equivalent
DQN	Deep Q-Network
GBRT	Gradient Boosting Regression Trees
IT	Information Technology
MAPE	Mean Absolute Percentage Error
MDP	Markov Decision Process
MED	Multi-Effect Distillation
ML	Machine Learning
MSE	Mean Squared Error
MSF	Multi-Stage Flash
R <sup>2</sup>	Coefficient of Determination
ReLU	Rectified Linear Unit

RL	Reinforcement Learning
RMSE	Root Mean Squared Error
RO	Reverse Osmosis
UAE	United Arab Emirates

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Paper submitted: 20.06.2025  
Paper revised: 21.12.2025  
Paper accepted: 04.01.2026