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Predicting energy performance of the drinking water treatment process and its determinants

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ABSTRACT

Within the global climate change framework, enhancing energy efficiency presents a significant challenge for water utilities. Drinking water treatment is energy-intensive, involving several physicochemical processes to remove multiple pollutants from raw water. This study employs artificial neural networks (ANNs) and decision tree methods to gain a deeper understanding of the water–energy nexus in drinking water treatment processes. The energy efficiency of a sample of Chilean drinking water treatment plants (DWTPs) was estimated, resulting in an average score of 0.343. This indicates that on average, DWTPs could potentially save 65.7% of their current energy consumption if they were operating at an efficient level while producing the same quantity and quality of drinking water. The main source of raw water and the technology for treating water have been identified as critical factors influencing energy efficiency. Specifically, using surface water for producing drinking water, energy efficiency can increase to 0.514, whereas using groundwater would regress energy efficiency to 0.240. The use of predictive tools such as ANNs provides relevant information to support decision-making processes for a transition toward a sustainable urban water cycle.

Key words: artificial neural networks, drinking water treatment, energy efficiency, operating characteristics, regression tree methods, water–energy nexus

HIGHLIGHTS

- A neural network was used to predict the energy efficiency of the drinking water treatment.
- The average energy efficiency estimated was 0.343.
- Technology for treating water significantly influences energy efficiency.

GRAPHICAL ABSTRACT

NOMENCLATURE

Parameter	Meaning
DWTPs	Drinking water treatment plants
DEA	Data envelopment analysis
ANNs	Artificial neural networks
RT	Regression tree
RF	Random forest
MSE	Mean squared error
ReLU	Rectified linear activation unit
PF	Pressure filtration
RGF	Rapid gravity filtering
CF–PF	Coagulation–flocculation and pressure filtration
CG-RGF	Coagulation–flocculation and rapid gravity filtering
FP	Full private water companies
CS	Concessionary water companies
SISS	Superintendencia de Servicios Sanitarios
StoNED	Stochastic non-parametric envelopment of data
n	Number of units
d_i	Desired output
y^{actual}	Actual output
EE	Energy efficiency
$\hat{y}$	Predicted output
y^{actual}	Actual output
ε	Error
k	Set of predictors
T	Number of sub-divisions
$\widehat{\mu_\tau}$	Average value of the predicted variable
R_τ.	Sub-division
m	Subset of predictors
V_w	Volume of potable water
P_{sin}	Concentration of pollutant ‘s’ in the influent
P_{sef}	Concentration of pollutant ‘s’ in the effluent

1. INTRODUCTION

The Sustainable Development Goals set by the United Nations encompass various critical objectives for global development. Goal 6 emphasizes the importance of ensuring access to safe, clean, and affordable drinking water for all people by 2030. At the same time, Goal 13 calls for urgent action to combat climate change and its adverse effects (UN 2015). Water treatment processes aimed at converting raw water into potable water are known to be energy-intensive activities. When combined with wastewater treatment, these activities account for approximately 6% of regional electricity consumption (Kenway *et al.* 2019; Liu & Mauter 2021). The significant energy demand in water treatment makes it crucial to address energy efficiency and explore sustainable practices to achieve the goals set by the United Nations.

The pursuit of efficient energy use in the drinking water treatment process holds numerous benefits for society, the economy, and the environment (An *et al.* 2018). From an economic standpoint, optimizing energy consumption can lead to cost-savings by reducing both energy and production costs. These savings can be passed on to consumers in the form of lower water tariffs, making safe and clean drinking water more affordable for the population (Ngobeni & Breitenbach 2021). Furthermore, substantial amounts of energy consumption in water treatment processes can be linked to higher levels of air pollution and greenhouse gas emissions (Rothausen & Conway 2011; Facchini *et al.* 2017; Beeftink *et al.* 2021). By adopting energy-efficient technologies and practices, the water sector can play a crucial role in minimizing its environmental impact and contributing to overall sustainability (Bukhary *et al.* 2020). Addressing these challenges has placed the measurement of energy efficiency in drinking water treatment at the forefront of the water–energy nexus agenda for researchers and policymakers (Ahmad *et al.* 2020; Huang *et al.* 2023).

In the past, numerous studies have been conducted to assess the energy intensity involved in providing water services (e.g., Sanders & Webber 2012; Wakeel *et al.* 2016; Zib *et al.* 2021; Sowby 2023), including drinking water treatment plants (DWTPs) (Yateh *et al.* 2024). It is important to highlight that energy consumption can vary significantly among different water treatment facilities, which can be attributed to various factors. These factors include the source of the raw water (Majid *et al.* 2020; Czernek *et al.* 2021), the technologies utilized for producing drinking water (Grzegorzek *et al.* 2023), and the quality of the raw water (Sowby & Burian 2017; Molinos-Senante & Sala-Garrido 2019). Because of those multiple factors influencing energy use in DWTPs, it is also relevant to assess their energy efficiency, i.e., assessing the potential reduction of energy required to provide the same level of service.[1]

After reviewing 93 studies assessing energy use in DWTPs, Yateh *et al.* (2024) concluded the need for a better understanding of the tradeoffs between energy use and water treatment efficiency. Actually, previous research on estimating the energy efficiency of DWTPs using a multi-criteria approach is limited (e.g., Maziotis & Molinos-Senante 2024; Molinos-Senante & Guzmán 2018; Molinos-Senante & Sala-Garrido 2018; Ananda 2019; Molinos-Senante & Maziotis 2022a; Amaral *et al.* 2023; Maziotis *et al.* 2023). These previous studies are characterized by using the data envelopment analysis (DEA) method to build the energy efficiency synthetic index. DEA compares inputs and outputs across different facilities to identify both the best and worst performers (Hwang *et al.* 2016). The linear programming techniques employed by DEA construct a piecewise frontier based on observed data, which means that it does not allow for predicting relationships between inputs and outputs (Nazari-Shirkouhi *et al.* 2023). This limitation restricts the ability to understand and forecast potential changes in energy efficiency for these facilities.

In contrast to the DEA method, artificial neural networks (ANNs) employ machine-learning algorithms to identify patterns in data and enhance model performance by comparing predicted outputs with observed data (Nandy & Singh 2021). ANNs are flexible mathematical models that do not require the specification of a functional form for the production function connecting inputs to outputs. Instead, they assume that this relationship is unknown (non-parametric) and nonlinear (Azadeh *et al.* 2007).

ANNs have demonstrated themselves as a viable alternative method for evaluating and predicting the efficiency of various units (Dmytro *et al.* 2018; Tomar *et al.* 2022; Luo *et al.* 2023). Despite the numerous

[1] As stated by Molinos-Senante & Sala-Garrido (2018), energy intensity refers to the amount of energy consumed (measured in kWh) per unit volume (m^3) of drinking water processed, typically expressed as kWh/m^3. On the other hand, energy efficiency is a synthetic index that takes into account various factors, including the quality of the raw water being processed, the volume of drinking water, and the energy needed for its treatment.

advantages of ANNs, their application in the water industry has been relatively limited (e.g., Wibowo & Alfen 2015; Nafi & Brans 2018; Molinos-Senante & Maziotis 2022b; Xia *et al.* 2022; Zhang *et al.* 2022), and they have never been utilized to predict the energy efficiency of DWTPs. This study aims to address this gap in the existing literature by exploring the use of ANNs for predicting DWTPs' energy efficiency. Furthermore, to gain insights into whether operating characteristics, such as the age of treatment facilities, influence the energy performance of DWTPs, this study incorporates several decision tree methods. These machine-learning techniques allow for the visualization of factors influencing efficiency and enable more reliable explanations and decision-making processes (Rebai *et al.* 2019; Nandy & Singh 2021).

Against this background, this study has two main objectives. Firstly, it aims to assess and forecast the energy efficiency of the drinking water treatment process using neural network techniques. Secondly, the study seeks to gain a deeper understanding of the factors influencing energy performance. The novelty of this research is underscored by two primary contributions to the literature. Firstly, it introduces a neural network approach to predict the energy efficiency of the drinking water treatment process. This represents a pioneering application of machine-learning techniques for evaluating energy performance in this specific context. Secondly, the study employs decision trees to uncover hidden relationships within the data, enabling predictions on how efficiency might be influenced by various operating factors. This unique integration of machine-learning methods not only enhances the predictive capabilities of the research but also elucidates the determinants of energy efficiency in the drinking water treatment process. Overall, this research significantly advances the existing literature by providing novel insights and practical applications for understanding and forecasting energy performance in DWTPs.

2. MATERIALS AND METHODS

2.1. Prediction of energy efficiency

The energy efficiency of DWTPs and their determinants is predicted by employing ANNs. The backpropagation neural network method, which is widely used for making predictions (Liang & Wu 2005; Tosun 2012), has been selected for this analysis. In this iterative process, the predicted output from the ANN model is compared with the actual output, and the difference between them generates an error. This error is then used to adjust the weights of interconnected neurons until the error is minimized, and the predicted ANN output closely matches the actual output (Kwon 2017).

To carry out this analysis, the dataset is randomly divided into two separate datasets. The first dataset served as the training dataset, where the ANN model is trained to generate in-sample results (Hanafizadeh *et al.* 2014; Zhu *et al.* 2020). The second dataset, known as the testing dataset, is used to assess the model's out-of-sample performance and make predictions (Liao *et al.* 2007). The efficiency scores derived from these predictions are then used for further analysis (Athnassopoulos & Curram 1996).

To determine the optimal architecture for the best ANN model, several aspects should be considered, including the number of neurons in hidden layers, the number of hidden layers, the activation functions for both hidden and output layers, and the learning rate (Kwon *et al.* 2016; Zhu *et al.* 2020). The number of neurons in hidden layers can be determined using cross-validation techniques, where the average minimum mean squared error (MSE) is used as a criterion (Celebi & Bayraktar 2008):

$$\mathrm{MSE} = \frac{1}{n}\sum_{i=1}^{n}(d_i - y^{\mathrm{actual}})^2 \tag{1}$$

where n is the number of units, y^{actual} is the actual output (energy consumed), and d_i is the desired output.

MSE is a measure of the model's performance, indicating how close the predicted values are to the actual values. A lower MSE value indicates better performance, as it means the model's predictions are more accurate and closer to the true energy consumption values (Tosun 2012).

Activation functions are mathematical equations that dictate the behavior of neurons in the hidden layers. Various activation functions can be used, such as logistic (sigmoid), rectified linear activation unit (ReLU), hyperbolic tangent (tan$h$), Maxout unit, and SoftMax, among others (Emrouznejad & Shale 2009; Kwon 2014, 2017; Tsolas *et al.* 2020). The mathematical formulation can be consulted in Hu *et al.* (2019), whereas Equation (2) shows the ReLU activation function, which was optimal in this case study. These functions shape the estimated output of the network and determine whether the output needs activation after receiving weights and biases. The activation function of the output layer is typically a linear function of the inputs through the weights and biases (Liao *et al.* 2007; Kwon 2017). The learning rate is a crucial parameter that governs how quickly or slowly the ANN model learns from the given problem.

$$f(x) = x^{+} = \max(0, x) = \frac{x + |x|}{2} = \begin{cases} x & \text{if } x > 0 \\ 0 & \text{otherwise} \end{cases} \tag{2}$$

where x is the input to a neuron (Hu *et al.* 2019).

After training the best ANN model using the training dataset and making predictions with the testing dataset, energy efficiency scores are estimated using a defined approach (Azadeh *et al.* 2007, 2010):

$$\mathrm{EE} = \frac{y^{\mathrm{actual}}}{\hat{y} + \max(\varepsilon)} \tag{3}$$

where EE denotes energy efficiency, $\hat{y}$ is the predicted (estimated) output, y^{actual} denotes the actual output, and ε is the error. In Equation (3), EE ranges between zero and one. A value of one signifies that the DWTP is operating at 100% energy efficiency. On the other hand, values lower than one denote inefficiency, and the magnitude of the deviation from one represents the potential for energy savings.

By individually applying Equation (3), all the facilities were evaluated, and the separate estimations of energy efficiency were obtained for each DWTP. This allows for a specific assessment of energy inefficiencies at the scale of each individual DWTP.

2.2. Environmental variables influencing energy efficiency

The subsequent phase of the analysis aims to identify potential operating characteristics and environmental variables that might influence energy efficiency at DWTPs. Additionally, the objective is to predict how efficiency could be impacted by these operating characteristics. To accomplish this, a regression tree (RT) model is constructed, with energy efficiency obtained from the ANN model serving as the predicted variable. The model uses a set of operating characteristics, such as the age of the plant facility and the type of treatment technology employed (more detailed information on these variables is available in the next section), as predictors.

The RT model seeks to uncover patterns and relationships within the data by recursively partitioning the dataset based on the chosen operating characteristics and environmental variables. It forms a decision tree-like structure, where each internal node represents a predictor variable and a split point, and each leaf node corresponds to a predicted value of energy efficiency based on the characteristics of the facility. The RT follows a top-down methodology in which the dataset is initially divided into smaller regions. These sub-divisions are further partitioned through recursive partitioning, involving categorical and/or continuous predictors (Nandy & Singh 2021). Within each sub-division, the mean value of the predicted variable is determined based on the observations within that region, minimizing the sum of squared errors (James *et al.* 2013).

An RT model takes the generic form (Rebai *et al.* 2019):

$$f(k) = \sum_{\tau=1}^{T} \widehat{\overline{\mu_{\tau}}} K_{(K \in R_{\tau})} \tag{4}$$

where k presents a set of predictors, T is the number of sub-divisions (regions), and $\widehat{\overline{\mu_{\tau}}}$ denotes the average value of the predicted variable that is calculated for each sub-division based on the observations that belong to each sub-division R_{τ}.

To enhance the predictive capability of the RT, we utilize a complementary decision tree technique known as random forest (RF). This approach combines decision trees with bootstrap methods, employing a bootstrap aggregation method to generate a combined prediction from individual decision trees, referred to as a forest (Nandy & Singh 2021). The predicted variable is obtained as an average of the predictions made by all the trees (Scornet *et al.* 2015; Genuer *et al.* 2017; Thaker *et al.* 2021).

RF predictions exhibit increased robustness and reduced sensitivity to outliers compared to other methods (Hallet *et al.* 2014). To ensure that there is no correlation among the trees, the following procedure is implemented. First, the RF algorithm selects a bootstrap sample randomly for training. Second, at each split, the algorithm randomly picks a subset of m predictors from the total set of k predictors. In the case of RF regressions, the default value for m predictors is defined as $m = k/3$ (Rebai *et al.* 2019). Lastly, the predicted variable is obtained by taking the average of predictions from all the trees (Thaker *et al.* 2021). This ensemble approach results in enhanced prediction accuracy and robustness. Similar to the RT, RF also provides a means to visualize the importance of predictors concerning the predicted variable. Predictors that yield higher values are considered more significant than others in influencing the outcome (Hallet *et al.* 2014; Thaker *et al.* 2021). This ranking of predictors based on their importance allows for a better understanding of the factors that have the most substantial impact on the model's predictions.

2.3. Case study: data sample and variable selection

The empirical application centers around the examination of 146 DWTPs situated in Chile. These facilities adopt various technologies for treating water before supplying it to consumers. The employed technologies encompass: (i) pressure filtration (PF); (ii) rapid gravity filtering (RGF); (iii) coagulation–flocculation and pressure filtration (CF–PF), and (iv) coagulation–flocculation and rapid gravity filtering. Unfortunately, data regarding the use of chemicals by each DWTP was not available. Nevertheless, all facilities meet the quality standards defined by the national Chilean drinking water law (NCh409/1).

From a management standpoint, all these DWTPs are operated by private water companies. During the 1998–2004 period, the water industry in Chile underwent privatization, resulting in the establishment of two types of water companies, namely full private (FP) water companies and concessionary (CS) water companies. This privatization approach was introduced to bring private sector participation and efficiency in the water sector (Ferro & Mercadier 2016).

Regardless of the type of water company operating the DWTPs, water is treated to adhere to high-quality standards established by the Ministry of Health of Chile. These standards are developed based on guidelines set forth by the World Health Organization (Molinos-Senante & Sala-Garrido 2018). The national regulator, Superintendencia de Servicios Sanitarios (SISS), was established with the purpose of overseeing and monitoring the economic and environmental performance of the water industry in Chile. By monitoring the industry's performance, SISS aims to safeguard consumer interests, promote transparency, and maintain the quality of water services while also addressing environmental concerns related to water treatment and distribution (Maziotis *et al.* 2023).

The selection of variables for this study was based on data availability and previous research conducted on this topic (Dong *et al.* 2017; Molinos-Senante & Guzmán 2018). Because the objective of the study is to predict the energy efficiency of DWTPs, the output of the ANN model is represented by the energy consumed by each facility measured in kilowatt-hours (kWh) per year, as demonstrated in previous studies. Regarding the inputs of the ANN model, they are specifically selected to represent the quality aspects of both the raw water treated in the DWTPs and the potable water generated. Consequently, quality-adjusted inputs are defined based on Equation (5) as a means to capture these relevant factors in the energy efficiency of the water treatment process (Walker *et al.* 2020). This approach ensures that the ANN model captures and considers the significant variables related to water quality and its treatment, ultimately contributing to a more accurate assessment of energy efficiency in the water treatment process.

$$\text{Quality adjusted water}_s = V_w \cdot \left(\frac{P_{\text{sin}} - P_{\text{sef}}}{P_{\text{sin}}}\right) \tag{5}$$

where V_w denotes the volume of potable water and is measured in m^3 per year, and P_{sin} and P_{sef} represent the concentration of pollutants P_s in the influent and effluent, respectively. Based on Maziotis *et al.* (2023) and Sala-Garrido *et al.* (2021), four pollutants are considered in the assessment: sulfates, turbidity, arsenic, and total dissolved solids. Considering data availability at the DWTP level for influent and effluent flows, four quality-adjusted inputs are used in this study. Nevertheless, other relevant parameters such as pH, conductivity, nitrates, and others would be relevant to include in the energy efficiency assessment if statistical information becomes available.

The study utilized the following variables to capture the operating characteristics of the drinking water treatment facilities: (i) *Age of DWTP*: this variable represents the age of the treatment facility and is considered a continuous variable, indicating the number of years since its establishment and (ii) *Main source of raw water*: this is a categorical variable that captures the source of water used by the treatment facility. It includes three categories: surface water, groundwater, and mixed water resources; (iii) *Main treatment technology*: this categorical variable is used to identify the specific treatment technology employed by the facilities. It encompasses four different types of technology, i.e., PF, RGF, CF–PF, and CF–RGF, and (iv) *Type of ownership*: This variable is represented as a dummy variable, taking the value 1 for FP water companies and 0 for CS water companies.

Table 1 summarizes the descriptive statistics of the variables that were provided by the SISS.

3. RESULTS AND DISCUSSION

3.1. Basics of the estimated ANN

The first stage in our analysis was to prepare the dataset for training and testing. In doing so, a data preprocessing analysis was conducted. The data were normalized using the min–max normalization process (Liao *et al.* 2007). Normalization ensures that all the input features are scaled to a similar range, preventing some variables from dominating the learning process due to their larger magnitudes (Wang 1996). Subsequently, the dataset was split into a 70:30 ratio, with 70% of the observations used for training the model and the remaining 30% for testing (Kwon 2017). This splitting allows the model to learn from a substantial portion of the data and then assess its performance on unseen data during testing, providing an indication of the model's generalization capability. Accordingly, energy efficiency was predicted for 44 DWTPs. Once the data preprocessing and splitting were completed, the ANN model could be trained using the training dataset (Table 2).

The best ANN model employed a specific architecture with one input layer, one hidden layer, and one output layer. The input layer had four neurons, each corresponding to the four quality-adjusted inputs defined in the previous section. According to past research (Patuwo *et al.* 1993; Azadeh *et al.* 2010; Kwon *et al.* 2016; Kwon 2017), the ANN model included one hidden layer that had nine neurons, which were determined to be optimal through cross-validation techniques (Liao *et al.* 2007; Celebi & Bayraktar 2008). The output layer consisted of one neuron, representing the energy consumption. The MSE (Equation (1)) of the ANN model was 0.012.

In the best ANN model, the activation function used for the neurons in the input layer was ReLU (Equation (2)). On the other hand, the activation function for the neuron in the output layer was the linear function. The linear function is a straightforward activation that returns the input value unchanged. For training the ANN model, the backpropagation algorithm was employed with a maximum of 1,000 iterations. Additionally, the

Table 1 | Descriptive statistics to predict the energy efficiency of DWTPs

Variables	Unit of measurement	Mean	Median	Std. Dev.	Minimum	Maximum
Energy consumed	kWh/year	148,049.85	60,713.23	195,323.32	1,152.32	1,054,754.23
Turbidity	m^3/year	2,294,674.23	1,347,533.43	3,027,762.10	3,126.22	11,538,685.45
Total dissolved solids	m^3/year	1,741,844.03	1,240,522.43	2,471,374.03	4,145.03	10,983,351.23
Sulfates	m^3/year	1,370,566.83	1,295,614.42	1,913,461.81	5,604.14	8,113,707.00
Arsenic	m^3/year	1,998,544.22	1,363,691.45	2,633,425.72	4,669.83	10,695,107.94
Age of plant	years	28.01	22.76	16.42	11.03	72.40

Note. Observations: 146.

Table 2 | Estimated parameters of the ANN

Network architecture	4–9–1
Activation function	ReLU/Linear
Algorithm	Backpropagation
Epochs	1,000
Learning rate	0.001
Mean squared error	0.012

learning rate used for the backpropagation algorithm was 0.001. A smaller learning rate leads to slower convergence but can help prevent overshooting the optimal solution (Di Martino *et al.* 2022).

Table 3 presents different metrics of error used to evaluate the performance of the generated ANN model during both the training and testing processes. These error metrics help assess the appropriateness of the ANN model for making predictions (Celebi & Bayraktar 2008; Kwon 2017).

3.2. Energy efficiency of DWTPs

Based on the analysis using the testing dataset ($n = 44$) and the predictions made by the ANN model, Figure 1 displays the energy efficiency scores for each evaluated DWTP. The results indicate that the drinking water treatment process in the studied DWTPs was characterized by high levels of energy inefficiency. This means that the energy consumption in the water treatment process was relatively high compared to the ideal energy-efficient scenario. The mean energy efficiency score obtained from the predictions is reported as 0.343. Interpreting this value implies that, on average, the potential savings in energy consumption among the DWTPs could be as high as 65.7%. In other words, there is considerable room for improvement in energy efficiency, and by implementing more efficient practices, the DWTPs could potentially reduce their energy consumption significantly.

The results obtained in this current study demonstrate consistency with the energy efficiency estimates obtained from other methodologies used in past research. Maziotis *et al.* (2023) utilized DEA models to estimate average energy efficiency for the DWTPs. They reported an average energy efficiency of 0.163 based on a common set of weights and 0.329 when flexible weights were allocated. Sala-Garrido & Molinos-Senante (2020) used the DEA tolerance model to estimate energy efficiency and provided a slightly larger average of 0.43 for the Chilean facilities. Molinos-Senante & Maziotis (2022a) applied the stochastic non-parametric envelopment of data method to a sample of Chilean facilities, resulting in an estimated average energy efficiency of 0.432. Overall, the consistency of the results across various research methodologies highlights the energy inefficiency challenges faced by the drinking water treatment sector in Chile.

Table 3 | Error metrics to evaluate the performance of the ANN

	Mean squared error	Root mean squared error	Mean absolute error
Training	0.015	0.121	0.091
Testing	0.012	0.112	0.096
Cross-validation	0.017	0.1295	0.879

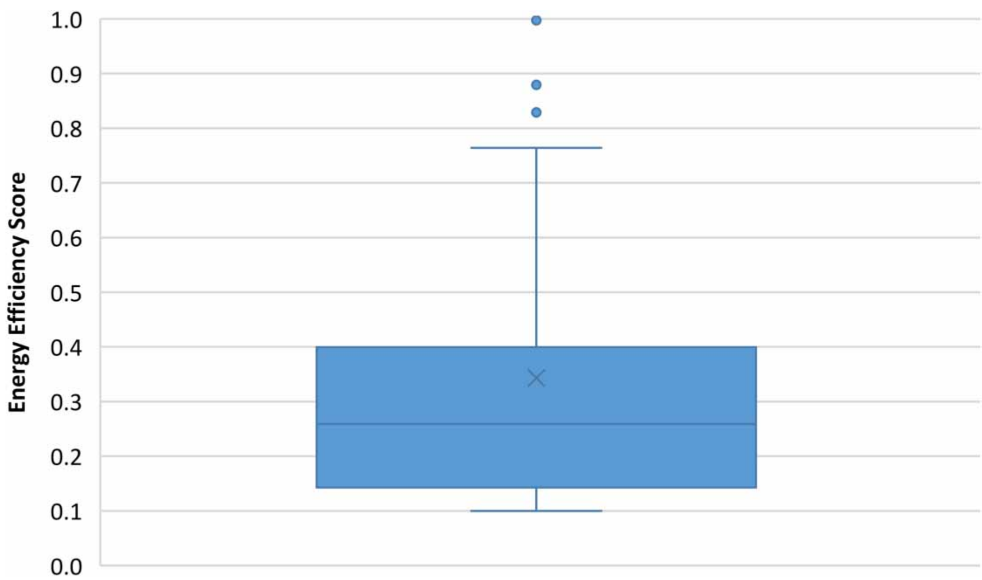

Figure 1 | Statistics of energy efficiency predictions on evaluated drinking water treatment plants.

Figures 1 and 2 indeed highlight significant disparities in energy efficiency among the evaluated DWTPs. The energy efficiency scores vary widely, indicating varying levels of energy optimization in the water treatment process. The DWTP with the lowest energy efficiency score at 0.10 implies that it would need to reduce its energy consumption by a substantial 90% to achieve a more efficient level of producing drinking water. Conversely, the most energy-efficient DWTP achieved a perfect efficiency score of 1.00, representing 100% efficiency. This indicates that the facility has optimized its water treatment process to minimize energy consumption and is operating at the highest level of energy efficiency achievable.

The DWTP with the highest energy efficiency score is a relatively small facility, treating approximately 85,000 cubic meters of water per year. This facility utilizes the CF-PF technology and has the advantage of being able to use both groundwater and surface water as water sources. This flexibility in water sources allows the water company to optimize its energy efficiency by choosing the most energy-efficient water source depending on various factors such as availability and energy requirements. Conversely, the DWTP with the lowest energy efficiency score, despite using the same CF-PF technology as the most energy-efficient facility, treats a significantly smaller volume of water, only 1,100 cubic meters per year. This smaller scale of operation can limit the adoption of economies of scale advantages that larger facilities might enjoy. As a result, the facility faces challenges in achieving high energy efficiency, given the inherent limitations in its water treatment process and energy usage.

These differences in facility size, water volume treated, and the availability of multiple water sources showcase the complex interplay of factors that influence energy efficiency in the drinking water treatment process (see Section 3.3). Understanding these specific characteristics helps water utility managers and policymakers identify opportunities for improvements in energy efficiency for each facility and can guide strategic decisions to optimize energy usage across the DWTPs.

The substantial divergence in energy efficiency levels observed across the DWTPs analyzed demonstrates that some facilities have already implemented effective energy-saving measures, while others have significant opportunities for improvement. This highlights the importance of identifying and implementing energy-efficient practices in the water treatment sector to reduce overall energy consumption and its associated environmental impact. Some improvement opportunities are as follows: (i) *Optimize pumping systems*: pumps are one of the most energy-intensive components in water treatment plants (Bukhary *et al.* 2020). Ensure that pumps are properly sized, and use variable frequency drives to match pump output with the demand; (ii) *Implement process automation*: integrate process automation and control systems to optimize water treatment processes. Automation can respond to changing demand and water quality, ensuring processes run at the most energy-efficient levels (Musabandesu & Loge 2020); (iii) *Renewable energy integration*: consider integrating renewable energy sources, such as solar panels or wind turbines, to power certain aspects of the treatment process. Renewable energy can offset some of the plant's electricity needs (Sowby 2023); (iv) *Regular maintenance*: implement a

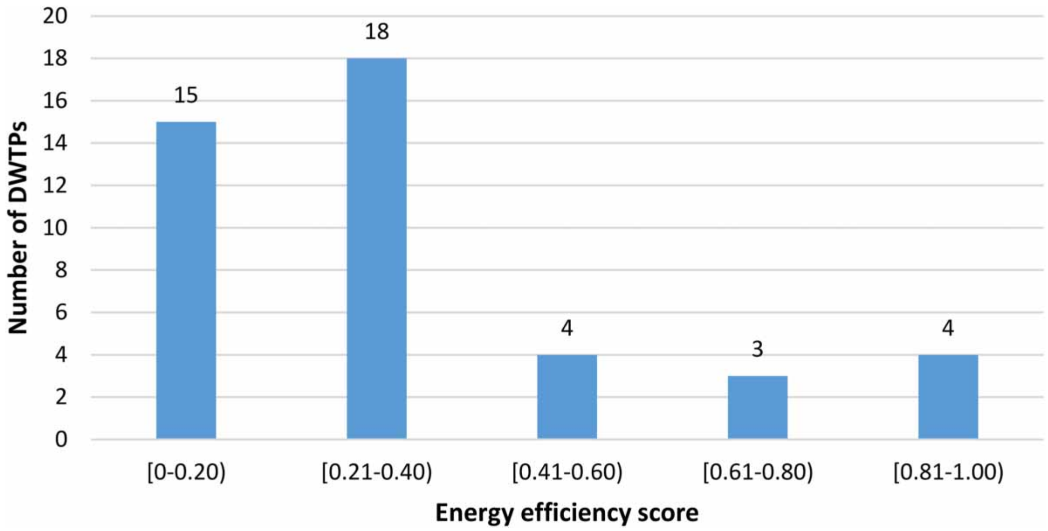

Figure 2 | Histogram with the distribution of energy efficiency scores.

comprehensive maintenance program to keep equipment running optimally. Well-maintained equipment operates more efficiently and has a longer lifespan (Wilson *et al.* 2021).

3.3. Influence of operational and environmental variables on the energy efficiency of DWTPs

Figure 3 represents the results from the RT analysis, which aims to understand the role of different operating characteristics on energy efficiency in the DWTPs. The RT utilizes the energy efficiency score obtained from the ANN model as the predicted variable and includes four predictor variables related to the DWTPs' operating characteristics: age of the facility; technology; source of raw water; and ownership. Each branch of the tree corresponds to a specific combination of predictor variables. The tree splits the data into subsets based on these characteristics and displays the average predicted energy efficiency score at the bottom of each branch. The 'left' branch of the tree indicates the results for the subset of observations that satisfy the condition in the node ('yes'). The 'right' branch represents the results for the subset of observations that do not satisfy the condition in the node ('no') (Rebai *et al.* 2019).

The findings of this study reveal that the energy efficiency of DWTPs is significantly influenced by two key factors: the source of raw water and the type of treatment technology used. The age and ownership of the treatment facility also play a role, although its impact on energy efficiency is relatively smaller as indicated by the variable importance values (see Supplementary Material). The results obtained from the RT analysis (Figure 3) suggest that if treatment facilities utilize surface water as their source, they might achieve an energy efficiency score of 0.514. In contrast, if facilities treat water from groundwater and mixed water resources, they might experience a notable drop in energy efficiency, reaching a score of 0.240. These findings highlight the critical role of the raw water source in determining the energy efficiency of DWTPs. They align with previous research investigating the water–energy nexus within the urban water cycle (Ahmad *et al.* 2020; Arfelli *et al.* 2022). Additionally, as water scarcity becomes more pronounced, the need for deeper wells arises to access water resources. However, drilling deeper wells involves higher energy intensity, leading to a decrease in energy efficiency. This highlights the challenge of balancing water availability with the energy required for extraction, a crucial consideration in sustainable water management strategies.

When focusing on the main technologies used for treating water, it becomes evident that certain treatment methods, such as PF and CF–PF, could result in higher energy requirements for water treatment. On average, the energy efficiency of DWTPs may decrease to 0.210 when these technologies are employed to remove pollutants from raw water sourced from groundwater and mixed resources. In contrast, the use of technologies like RGF and CF–RGF for water treatment could lead to a higher energy efficiency level of 0.280. Interestingly, these findings partially support the conclusions reached by Molinos-Senante & Sala-Garrido (2018), which also highlighted the significant influence of treatment technology on the energy performance of DWTPs. However, it should be noted that their results indicated both CF–PGF and CF–PF as the technologies exhibiting the best energy efficiency.

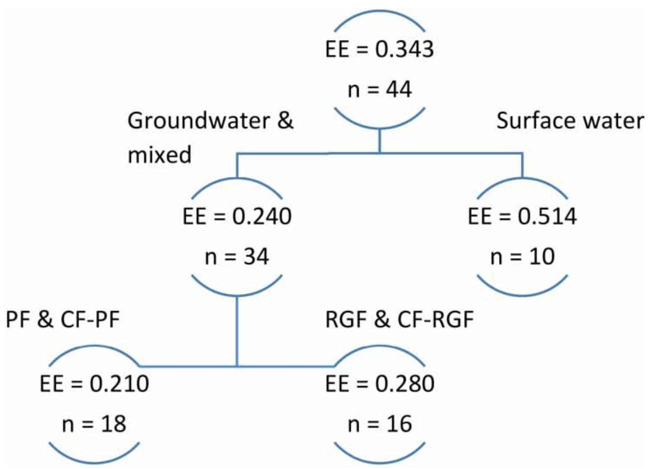

Figure 3 | RT results (the dependent variable is the energy efficiency score).

In the RF assessment, four predictors were used, and the optimal value of m (the number of predictors randomly selected for splitting at each node) was set to 1. To achieve stable regression results, the number of trees in the RF model was set to 3,000, following the approach proposed by Thaker *et al.* (2021). The minimum (optimal) number of trees was found to be 100, indicating that the RF regression achieved its best prediction performance when using 100 trees. This conclusion was based on the analysis of prediction errors, as shown in Supplementary Material, Figure S2.

The results from the RF tree are reported in Figure 4. At the bottom of each branch, the predicted average energy efficiency is indicated based on the observations of different predictors that belong to that subset. The results indicate that different types of water sources and the age of the treatment facility had a major influence on energy efficiency. The ranking of the importance values of each variable indicated that different types of treatment technologies also impacted efficiency. In contrast, the effect of ownership on energy efficiency was negligible (see Supplementary Figure S3 and Table S1).

The results obtained from the RF regression analysis indicate that water treatment plants can enhance their energy efficiency by opting to treat surface water. Similar to the findings from the RT analysis, this suggests that treating surface water might be less energy-intensive compared to treating water sourced from groundwater and mixed water resources. The average predicted energy efficiency for DWTPs treating surface water could reach a level of 0.559. On the other hand, if treatment plants use water from sources other than surface water and have a facility age of more than 42 years old, their energy efficiency could substantially decrease to 0.144. This highlights the potential challenges and energy inefficiencies associated with using alternative water sources and operating older treatment facilities. However, if the age of the treatment plant falls within the range of 29.5–42 years old, its energy efficiency could improve, reaching a level of 0.242.

Energy inefficiency emerges as a significant concern for water treatment plants that have been operating for less than 29.5 years and that treat either surface water or groundwater. The average energy efficiency for such plants could decline substantially, reaching as low as 0.109. Slightly higher levels of energy efficiency could be achieved for treatment plants that have been in operation for a period between 18.5 and 29.5 years and treat water sourced from mixed resources. These plants could potentially attain an average energy efficiency score of 0.131. This suggests that moderate improvements in energy efficiency are attainable for such facilities. In contrast, DWTPs with a facility age of less than 18.5 years and that treat water from mixed resources have the potential to achieve a much higher energy efficiency level, reaching 0.393. This indicates that newer plants using mixed water resources have a promising opportunity to significantly improve their energy efficiency performance.

These findings underscore the importance of considering the source of water and the age of treatment facilities in optimizing energy efficiency within water treatment processes. Choosing to treat surface water and upgrading

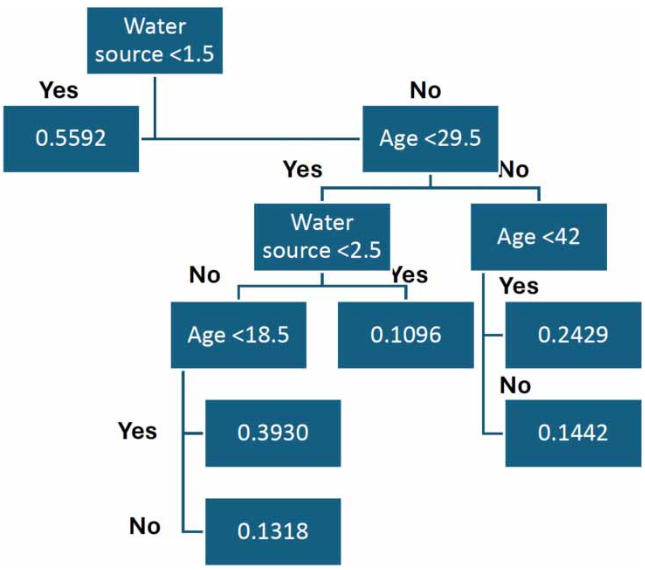

Figure 4 | Results of the random forest tree (the dependent variable is the energy efficiency score).

aging facilities could present valuable opportunities for improving energy performance and sustainability in water treatment operations. This information is highly valuable within the framework of the Energy Efficiency Directive (2023/955), which underscores the significance of promoting cost-effective energy efficiency measures and conducting energy audits in the water sector (European Union 2023).

4. CONCLUSIONS

Improving energy efficiency in providing drinking water services is crucial for effectively addressing multiple Sustainable Development Goals (SDGs). However, to achieve accurate efficiency estimations, robust approaches are essential. In this study, we introduce an innovative method by estimating energy efficiency scores of DWTPs using ANNs, which, unlike traditional non-parametric methods, enable predictions based on the nonlinear relationships between inputs and outputs.

The average energy efficiency of the assessed DWTPs was estimated to be 0.343, indicating that they could potentially save around 66% of their current energy use if they operated efficiently. Moreover, notable divergences were observed among the facilities, with 75% exhibiting an energy efficiency score lower than 0.4 and only 9% achieving an energy efficiency higher than 0.8. The impact of the source of raw water on energy efficiency was also evaluated, showing potential energy efficiency scores varying from 0.240 for groundwater to 0.514 for surface water. Beyond the specific results obtained from the case study, this research makes significant contributions to enhancing our understanding of the water–energy nexus within the urban water cycle. Firstly, it presents a robust technique for comparing and predicting the energy efficiency of the drinking water treatment process. Policymakers can rely on these results to draw informed conclusions about the energy inefficiency level in the industry. Secondly, by employing the RT and RF approaches to analyze the impact of operational variables on energy efficiency scores, specific targets for DWTPs can be defined. This allows for the development of more tailored and realistic measures for individual facilities to meet energy efficiency goals effectively. In conclusion, this study provides valuable insights and practical tools for advancing energy efficiency in the drinking water sector and contributes to broader efforts in achieving sustainable development goals.

While this study makes notable contributions to the literature within the water–energy nexus, it is not without limitations. From a methodological perspective, ANNs function as 'black-box' models, making it impossible to quantify the impact of each predictor on energy efficiency. However, by conducting several assessments integrating different quality-adjusted inputs, it is possible to identify the main drivers of energy efficiency in DWTPs. Additionally, ANNs require large amounts of data to avoid overfitting, which can be a limitation when the number of DWTPs to be evaluated is relatively small, not as in this case study, which evaluates 146 DWTPs. Finally, due to data availability restrictions, only four quality-adjusted inputs were used as energy efficiency predictors. Therefore, it would be desirable to integrate additional quality parameters that might influence the energy efficiency of DWTPs.

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DATA AVAILABILITY STATEMENT

Data cannot be made publicly available; readers should contact the corresponding author for details.

CONFLICT OF INTEREST

The authors declare there is no conflict.

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