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International Journal of Artificial Intelligence and Machine Learning

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AI-Driven Optimization of Wastewater Treatment Processes for Sustainable Environmental Management

Vikrant Gautam[1], Reshu Singh[2], Anusha Rani[3], Ranajeet Kumar[4], Ozair Ahmad[5], Sonu Kumar[6]

[1]Assistant Professor, Department of Civil engineering, Government Engineering College, Bhojpur. E-mail: vikrantgautamaara@gmail.com
[2]Assistant Professor, Department of Civil engineering, Government Engineering College, Bhojpur, School of Water Resources, Indian Institute of Technology, Kharagpur. E-mail: reshusingh5794@gmail.com
[3]Assistant Professor, Department of Civil engineering, College - Governmental Engineering College, Buxar, E-mail: anusha06.iitr@gmail.com
[4]Assistant Professor, Department of Civil Engineering, Sershah Engineering College, Sasaram, Department of Architecture and Regional Planning, IIT Kharagpur. E-mail: kumarranajeet@gmail.com
[5]Assistant Professor, Department of Electronics and Communication Engineering, Government Engineering College, Kishanganj. E-mail: ozair0590@gmail.com
[6]Assistant Professor, Department computer science and engineering, Government Engineering College Gopalganj.
E-mail: sonukumar2011998@gmail.com

Abstract
Wastewater treatment plants are subjected to continuously varying hydraulic and pollutant loads, while treatment performance, energy consumption and environmental impact must be maintained. This study presents an artificial-intelligence-based framework consisting of a predictive machine learning procedure and a constrained multi-objective optimisation for the adaptive operation of activated-sludge wastewater treatment. A BSM1-inspired synthetic benchmark comprising 16,128 operating observations was generated that encompass variations in influent flow, chemical oxygen demand (COD), total nitrogen (TN), ammonium nitrogen (NH4-N), temperature, dissolved oxygen (DO) set-point, internal recycle ratio, sludge retention time (SRT) and return activated sludge ratio. Multiple linear regression, random forest, Extra Trees and XGBoost models were assessed for the prediction of specific energy demand and effluent-quality indicators. XGBoost provided overall best predictive performance with an R^2 of 0.995 for energy demand, 0.948 for effluent COD, 0.970 for TN, 0.987 for NH4-N and 0.981 for the combined effluent-quality index (EQI). The trained XGBoost surrogate was coupled to a constrained particle swarm optimisation routine that identified operating set-points resulting in lower energy consumption without compromising effluent quality. When applied to 120 unseen influent conditions, the proposed framework reduced simulated specific energy demand from 0.462 to 0.358 kWh m−3 (22.5%) while decreasing COD, TN, NH4-N and the relative EQI by 7.3, 8.3, 2.8 and 9.7%, respectively. DO set-point and SRT were identified as the major controllable variables. The results demonstrated the effectiveness of integrating predictive modeling with prescriptive optimization to achieve energy-efficient and environmentally sustainable wastewater treatment. The study was conducted as a simulation-based proof of concept and requires validation on a long-term plant data basis prior to implementation.

Keywords: artificial intelligence; wastewater treatment; machine learning; XGBoost; particle swarm optimisation; aeration energy; sustainable environmental management; process control

1. Introduction

Wastewater treatment is a central pillar of public health, aquatic ecosystem protection, and water resource recovery. Modern wastewater treatment plants (WWTPs), however, are not simply passive purifiers. They represent highly complex, nonlinear and disturbance-driven process networks, in which influent flow, organic loading, nutrient concentrations and temperature change dynamically. Operators have to adapt to these disturbances, while achieving discharge quality and controlling electricity, pumping, aeration, sludge handling and chemical consumption. The resulting operating problem is inherently multi-objective: a control action that improves nitrification may augment aeration demand, while aggressive energy reduction may compromise ammonia removal or process stability.Aeration is particularly important since it is among the major energy consumers, as well as a critical variable for biological carbon and nitrogen removal. Recent reviews report that aeration can account for roughly half of treatment energy in many activated-sludge facilities, making dissolved oxygen control one of the most attractive targets for intelligent optimisation [1,2]. Conventional fixed set-points and proportional-integral control remain widespread since they are reliable and interpretable but are not designed to learn nonlinear interactions from historical sensor data. Artificial intelligence (AI) and machine learning (ML) offer complementary capability by learning complex input-output relationships, creating soft sensors, predicting effluent quality, detecting abnormal operation and supporting adaptive control [3-6].Research on learning-based models has progressed from isolated prediction-focused studies toward combined predictive-prescriptive systems. Deep-learning models have been applied to predict effluent outflows in real time, while reinforcement-learning and hybrid optimisation approaches have been successfully tested in terms of energy and cost reduction in representative or pilot-scale treatment systems [7–11]. That being said, several relevant research directions have been left underexplored. For example, while many works focus on predicting a certain target output (energy, nutrients, etc.), few propose actionable set-points based on the predicted outcomes. Additionally, while advanced control agents have been proposed, their training and safe deployment in real-world settings with limited digital infrastructure can be non-trivial. A practical control framework should therefore allow operators to reason on the predicted effects of candidate set-points before actual application.

This study addresses that need via a hybrid structure in which an ensemble gradient-boosting model acts as a fast surrogate of treatment behavior and a constrained particle swarm optimisation (PSO) layer searches for improved operating set-points. The principal aims are: (i) to compare representative statistical and tree-based ML models for energy and effluent-quality prediction; (ii) to quantify the predictive performance of the best-performing model; (iii) to use the learned model to optimise DO, internal recycle and SRT under unseen influent conditions; and (iv) to interpret the sustainability implications of the resulting operating strategy. Because no plant dataset was supplied for the present study, the numerical experiment is intentionally framed as a BSM1-inspired synthetic benchmark rather than as a full-scale plant validation. This distinction preserves methodological transparency while still allowing the proposed AI architecture to be tested reproducibly.

2. Related Work and Research Gap

2.1 AI applications in wastewater treatment

Current applications of artificial intelligence (AI) in wastewater treatment are focused on influent prediction, soft sensing, effluent quality prediction, membrane fouling prediction, energy management, anomaly detection, and process control. Broad reviews of these topics have been conducted by Safeer et al. [3], Wang et al. [4] and Zhang et al. [5]. Their main finding is a shift towards ensemble learning, deep learning, and hybrid optimisation; replacing classical artificial neural networks and fuzzy systems. The main reason for this shift is that biological treatment processes are better approximated through non-linear relations. While data-driven models can learn such relations directly from data, their performance depends on the quantity and quality of the data, as well as the similarity between training and deployment conditions.

Prediction accuracy has been significantly improved by modern architectures. Xie et al. [7] combined temporal convolutional networks with long short-term memory units to perform real-time effluent forecasting and demonstrated the importance of temporal feature extraction. Yang et al. [8] proved that optimised deep-learning architectures can outperform individual random forest, LSTM, convolutional and gated recurrent models for effluent prediction. Recent studies have also compared the performance of recurrent and gradient-boosting models for plant energy forecasting and highlighted the benefit of learning from long operational histories [12]. These works prove the predictive capabilities of ML, but operational value of a model depends on whether its predictions can be converted into controllable decisions.

2.2 From prediction to control and optimisation

Advanced control research has increasingly focused on AI-enabled optimisation. Croll et al. [9] systematically evaluated reinforcement-learning algorithms on a BSM1 treatment environment and reported that a twin-delayed deep deterministic policy-gradient agent could reduce aeration and pumping energy while maintaining treatment requirements. Later multi-objective reinforcement-learning work expanded the number of controlled actions and demonstrated the value, as well as the increased training complexity, of broader control authority [10]. Mao et al. [11] combined prediction and optimisation for aeration-energy reduction, while Achraf et al. [13] proposed an ensemble-based energy optimisation framework that generated actionable operating recommendations. These studies illustrate an important direction: AI is most useful when it moves beyond forecasting and supports decisions under explicit performance constraints.

The present work uses that predictive-prescriptive paradigm, but with a slightly more transparent architecture. In contrast to directly learning a control policy, the paper first trains and evaluates the plant surrogate, which is subsequently queried by the optimisation algorithm to determine candidate set-points. The benefit of this approach is two-fold: The model can be more easily audited, retrained, or reviewed by an operator and the optimisation process itself can be steered towards feasible or compliant solutions by incorporating domain-specific costs and penalties.

The contribution of the present work is therefore not the individual introduction of PSO or XGBoost, but rather the joint proposition to use those tools jointly as a tractable and interpretable means to tackle a multi-output optimisation of the treatment quality and consumption of energy in the framework of a single decision-support paradigm.

3. Materials and Methods

3.1 Benchmark design and data generation

Benchmark Simulation Model (BSM1) is a standard created to investigate activated-sludge control strategy under different influent circumstances [14]. The main idea was to compare various approaches with each other based on a particular set of process structures and performance indicators. In this research, a BSM1-like synthetic benchmark was constructed, which aimed to demonstrate common nonlinear characteristics related to AI-model development, but it cannot be regarded as the implementation of the BSM1 simulator itself. The reason for it was that the user did not provide any plant historian data or calibrated mechanistic model.

A total of 16,128 observations were generated, corresponding to the scale of twelve repeated 14-day dynamic operating blocks sampled at 15-minute resolution. The synthetic operating space encompassed hydraulic, organic and nutrient disturbances and controllable operating variables. Influent flow varied from 10,000 to 34,000 m3 d−1; influent COD varied from 220 to 800 mg L−1; influent NH4-N varied from 15 to 70 mg L−1; total nitrogen varied from 30 to approximately 100 mg L−1; and wastewater temperature varied from 10 to 30 °C. Controllable variables included DO set-point (0.8-3.0 mg L−1), internal recycle ratio (1.5-5.0), SRT (8-25 d) and return activated sludge ratio (0.5-1.2). Nonlinear response functions were employed to construct physically plausible dependencies: higher DO and SRT enhanced nitrification; recycle promoted nitrogen removal; high hydraulic loading decreased the effective treatment; and aeration, recycle pumping and solids handling increased energy demand. Gaussian disturbance terms were incorporated to avoid deterministic model fitting.

Table 1. Input and output variables used in the AI framework

Variable	Unit	Range / role	Interpretation
Influent flow	m3 d-1	10,000-34,000	Hydraulic disturbance
Influent COD	mg L-1	220-800	Organic loading
Influent NH4-N	mg L-1	15-70	Ammonia loading
Influent TN	mg L-1	30-100	Total nitrogen loading
Temperature	°C	10-30	Biological-rate modifier
DO set-point	mg L-1	0.8-3.0	Aeration control
Internal recycle ratio	-	1.5-5.0	Anoxic nitrate recycle
SRT	d	8-25	Biomass retention
RAS ratio	-	0.5-1.2	Secondary-settling return
Specific energy	kWh m-3	Model output	Energy objective
Effluent COD/TN/NH4-N	mg L-1	Model outputs	Quality objectives
Relative EQI	index	Model output	Combined environmental objective

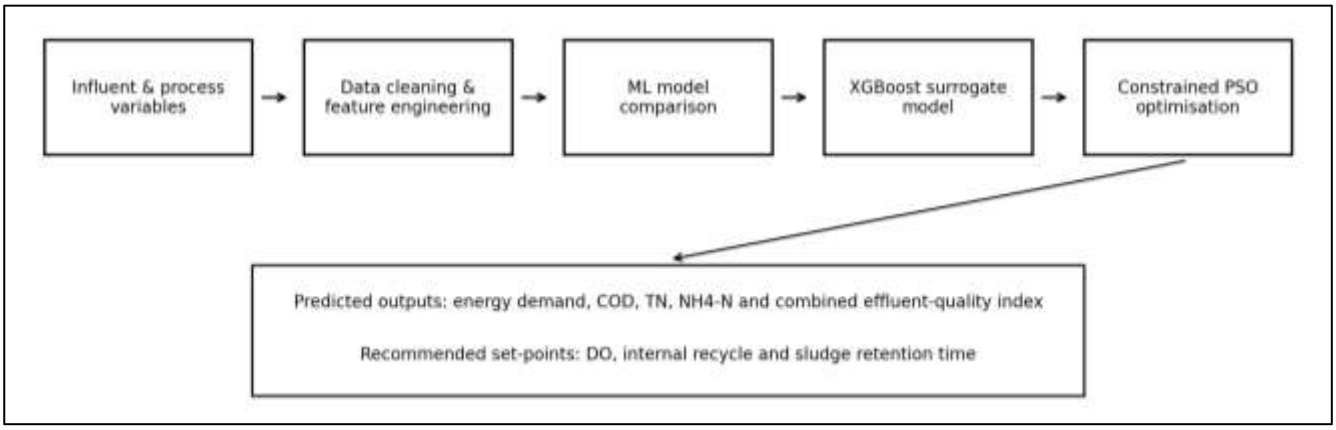

Figure 1. Predictive-prescriptive workflow of the proposed AI-driven wastewater optimisation framework.

3.2 Data preprocessing and partitioning

The resulting data set was pre-processed to remove missing values, duplicates and physically unrealistic values before model training. No feature standardisation was performed, since tree-based algorithms are not sensitive to the scale of the input data. Original engineering units were retained for the random forest, Extra Trees and XGBoost algorithms. An 80:20 random split was made to form training and hold-out test sets, with the latter not being used during parameter tuning. Model performance was quantified using the coefficient of determination (R^2), root mean squared error (RMSE) and mean absolute error (MAE). The five targeted outputs were specific energy demand, effluent COD, effluent TN, effluent NH4-N and relative EQI.

3.3 Machine-learning models

Four model families were compared. Multiple linear regression provided an interpretable baseline. Random forest represented bagged decision trees which reduced the variance through ensemble averaging. Extra Trees increased the tree randomisation and was included as it often performs well on tabular environmental datasets. XGBoost represented sequential gradient boosting with regularisation, row subsampling and feature subsampling. The XGBoost models used 420 boosting estimators, maximum tree depth of 6, learning rate of 0.05, subsample ratio of 0.85 and column-sampling ratio of 0.90. Separate XGBoost regressors were fitted for each output as a means of preserving error structures.

For an observed target yi and model estimate ŷi, prediction performance was quantified as follows: RMSE = $\text{sqrt}[(1/n)\Sigma(yi-\hat{y}i)^2]$, MAE = $(1/n)\Sigma|yi-\hat{y}i|$, and $R^2 = 1 - [\Sigma(yi-\hat{y}i)^2 / \Sigma(yi-\bar{y})^2]$. A lower RMSE or MAE indicates smaller prediction error, while an R^2 closer to one indicates that the model explains a larger proportion of target variability.

3.4 Constrained particle swarm optimisation

After model comparison, the best performing learner was used as a fast surrogate within a particle swarm optimisation routine. For each unseen influent condition, the optimiser varied three controllable variables: DO set-point, internal recycle ratio and SRT. Bounds were restricted to 0.8-3.0 mg L^{-1} for DO, 1.5-5.0 for recycle ratio and 10-20 d for SRT. The return activated sludge ratio was held at 0.8 so that the optimisation problem remained focused on three high impact decisions. A fixed baseline of DO = 2.2 mg L^{-1}, recycle ratio = 3.0 and SRT = 14 d was evaluated for the same influent conditions.

The objective function was composed of a weighted sum of normalised specific energy and normalised EQI. Penalty terms were added whenever the predicted value of COD, TN or NH_4-N exceeded 101% of their respective baseline prediction. Thirty particles were used for 28 iterations. The velocity of each particle comprised an inertial term plus a cognitive attraction term leading towards the particle's personal best solution and a social attraction towards the global best solution. This was an explicitly constrained formulation to prevent the undesired consequence of saving energy at the expense of deterioration in treated-water quality.

Algorithm 1. AI-driven set-point optimisation

Input: current influent/process vector x and trained XGBoost models
1. Set fixed baseline controls and predict baseline energy and effluent quality.
2. Initialise particles within feasible bounds for DO, recycle ratio and SRT.
3. For each particle, query the ML surrogate for energy, COD, TN, NH4-N and EQI.
4. Compute weighted energy-quality objective and add constraint penalties.
5. Update personal-best and global-best particle positions.
6. Update particle velocities and bounded positions.
7. Repeat Steps 3-6 for the specified number of iterations.
Output: recommended operating set-points and predicted performance improvement.

4. Results

4.1 Predictive performance

Table 2 summarises hold-out performance. XGBoost was generally the most accurate model for all five targets. The energy model achieved $R^2 = 0.995$ with RMSE = 0.009 kWh m^{-3}, while the NH_4-N model reached $R^2 = 0.987$ with RMSE = 0.803 mg L^{-1}. The prediction of the relative EQI was also satisfactory ($R^2 = 0.981$). The linear model was unexpectedly competitive for energy because the synthetic energy relationship includes a strong monotonic component, but it had much poorer accuracy for effluent quality. Random forest and Extra Trees provided useful baseline non-linear models, but XGBoost typically captured the interactions between load, temperature and set-points more accurately.

Table 2. Hold-out test performance of the candidate prediction models

Model	Target	R^2	RMSE	MAE
Multiple Linear Regression	Energy	0.989	0.012	0.010
Multiple Linear Regression	Effluent COD	0.902	5.096	4.040
Multiple Linear Regression	Effluent TN	0.934	1.645	1.297
Multiple Linear Regression	Effluent NH4-N	0.921	1.968	1.489
Multiple Linear Regression	EQI	0.924	6.113	4.734
Random Forest	Energy	0.910	0.035	0.027
Random Forest	Effluent COD	0.911	4.852	3.773
Random Forest	Effluent TN	0.878	2.242	1.738
Random Forest	Effluent NH4-N	0.932	1.828	1.375

Random Forest	EQI	0.932	5.810	4.333
Extra Trees	Energy	0.945	0.027	0.021
Extra Trees	Effluent COD	0.922	4.559	3.530
Extra Trees	Effluent TN	0.895	2.078	1.611
Extra Trees	Effluent NH4-N	0.952	1.527	1.147
Extra Trees	EQI	0.949	5.039	3.729
XGBoost	Energy	0.995	0.009	0.007
XGBoost	Effluent COD	0.948	3.730	2.961
XGBoost	Effluent TN	0.970	1.106	0.872
XGBoost	Effluent NH4-N	0.987	0.803	0.616
XGBoost	EQI	0.981	3.101	2.388

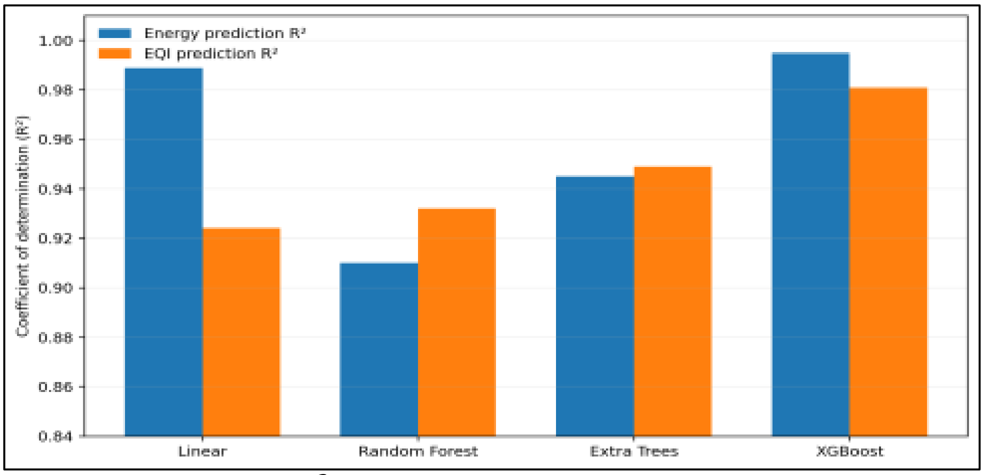

Figure 2. Comparison of R^2 for energy and combined effluent-quality prediction.

4.2 Feature influence and process interpretation

Mean feature-importance analysis across the five XGBoost outputs revealed that DO set-point was the most important variable (importance 0.383), followed by SRT (0.196) and influent TN (0.136). Temperature, influent COD and influent NH4-N formed a secondary group of process influential factors. The predominance of DO is to be expected from an activated-sludge process perspective, as it modulates both substrate oxidation and nitrification, while aeration is an energy-intensive process. SRT determines the retention of slower-growing nitrifying bacteria and has an impact on solids management, and the result therefore suggests that the model had captured some domain knowledge, learning not only about influent load dependencies but also about controllable process variables that could benefit from optimization.

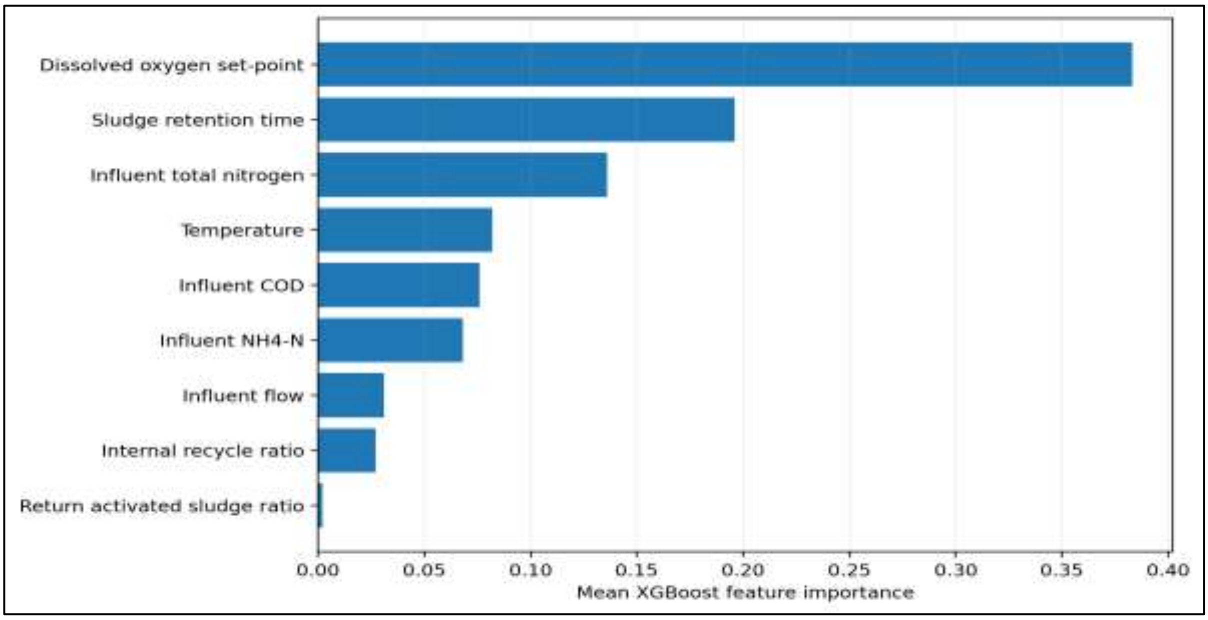

Figure 3. Mean XGBoost feature importance across the five predicted outcomes.

3.3Optimisation performance

The 1972ptimizer1972on stage has been tested on 120 unseen influent conditions. Table 3 compares the fixed baseline operation with AI-optimised set-points. The average specific energy demand has been reduced by 22.5% (from 0.462 to 0.358 kWh m −3). Moreover, the energy reduction has not been achieved at the expense of worse effluent quality. Indeed, a decrease in predicted COD (7.3%), TN (8.3%) and NH 4-N (2.8%) has been observed, resulting in an overall reduction in the relative EQI of 9.7%. The mean 1972ptimizer controls were DO = 1.63 mg L −1, internal recycle ratio = 2.49 and SRT = 19.99 d. The relatively low variation of the selected SRT suggests that the 1972ptimizer systematically preferred the upper part of the practical SRT range, which, by increasing the nitrification robustness, compensated the lower aeration set-point.

Table 3. Baseline and AI-optimised performance across 120 unseen operating conditions

Metric	Baseline	Optimised	Change (%)
Specific energy (kWh m-3)	0.462	0.358	-22.5
Effluent COD (mg L-1)	52.789	48.940	-7.3
Effluent TN (mg L-1)	28.599	26.230	-8.3
Effluent NH4-N (mg L-1)	9.462	9.197	-2.8
Relative effluent quality index	76.076	68.666	-9.7

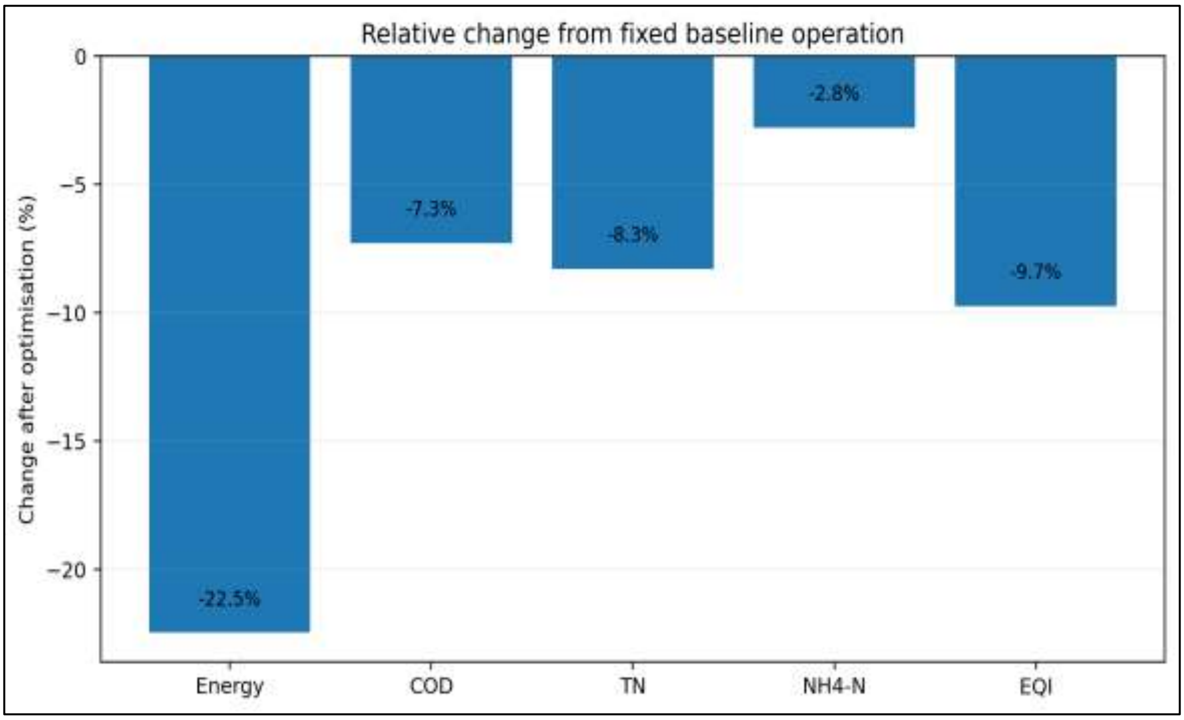

Figure 4. Percentage change in energy and effluent metrics after constrained optimisation.

5. Discussion

5.1 Significance of the predictive-prescriptive architecture

The central finding is that accurate tabular ML predictions could be translated into operational recommendation without having to rely on end-to-end black-box control agent. The nonlinear relationships learned by the XGBoost surrogate were sufficient to allow rapid exploration of a large set of potential candidate set-points. This was an attractive proposition for WWTPs where optimisation could be performed in an advisory mode prior to implementation of a closed-loop control strategy. The operators could then examine the recommended DO, recycle and SRT values, in conjunction with their predicted consequences for energy and effluent quality. This could provide a more easily validated route to control than direct reinforcement-learning control, particularly if process data from the plant were sparse or if regulatory oversight required an explicit operator in the loop.

The 22.5% simulated energy reduction is consistent with the general literature trend, though a direct comparison of numbers should be made cautiously, due to different process configurations, energy accounting and constraints. Croll et al. [9] reported a 14.3% reduction in aeration and pumping energy for their best RL configuration, compared to BSM1 benchmark control. Mao et al. [11] reported a higher aeration-energy reduction, using a coupled AI model, while recent energy-optimisation studies have shown that savings can be significant when flexibility and data quality are high [13]. The present results are therefore within a possible range for a simulation study, but should not be interpreted as a guaranteed full-scale saving.

5.2 Sustainability implications

Energy efficiency in wastewater treatment has environmental impacts beyond electricity costs. Reduced aeration and pumping demands can avoid indirect greenhouse-gas emissions in cases where the electricity supply is carbon intensive. Enhanced nitrogen and ammonia removal also reduces the eutrophication pressure on the receiving waters. In a broader sustainable-management context, AI-enabled operation can contribute to the achievement of SDG 6 (enhanced water quality), SDG 9 (digital and intelligent infrastructure) and SDG 12 (more efficient use of energy and treatment resources). Recent literature on carbon-neutral wastewater treatment also highlights the role of AI in the co-ordination of energy, emissions, chemical use and resource recovery [15,16].

Table 4. Sustainability contributions and practical indicators

Sustainability dimension	AI-enabled mechanism	Operational indicator
Energy efficiency	Adaptive DO and recycle set-points	kWh per m3 treated
Water-quality protection	Prediction and constrained optimisation of COD/TN/NH4-N	Effluent concentration and EQI
Carbon mitigation	Reduced electricity requirement and carbon-aware scheduling	kg CO2-e per m3, where grid factor is available
Resource efficiency	Coordinated SRT and solids-management decisions	Sludge production and handling energy
Operational resilience	Early prediction under changing influent conditions	Violation frequency and recovery time
Digital governance	Explainable recommendations and audit trail	Operator acceptance, override rate, model drift

5.3 Practical implementation pathway

A plausible rollout would involve getting history involved before full autonomy. Online sensors for flows, DO, ammonia, nitrogen, temperature, and basic water-quality variables would be synchronized with lab results and data about energy meters. The predictive model would be trained up on at least a seasons' worth of data (if possible) and include proper handling of sensor downtimes, maintenance periods, and process regime changes. The recommendations would initially be issued as operator decision-support aids. Once sufficient validation had occurred in shadow-mode, the recommended set-points could then be written to the supervisory control system, subject to hard safety limits and manual override. Model-drift detection should be performed to trigger retraining when prediction errors exceed acceptable thresholds.

Explainability is another essential feature. Feature importance, local sensitivity analysis, and counterfactuals allow for the interpretation of the reason for recommendation changes. For example, a decrease in the recommended DO recommendation is always associated with an increase in the predicted ammonia risk for the current load. Cybersecurity and data governance must be integrated into the system as engineering requirements. Access control, network segmentation, authenticated model updates, versioning, and rollback features are necessary for AI systems making recommendations to critical infrastructure software.

6. Limitations and Future Work

The main limitation of this study is that a synthetic, BSM1-based benchmark, not a calibrated, large-scale WWTP data set, was utilized. Although the former was engineered to contain realistic, non-linear trends and hiccups, it fails to account for all biochemical interactions and sensor bias, equipment limitations or seasonal pattern. As such, the reported numerical improvements are algorithmic feasibility rather than guaranteed field performance. A second limitation is the lack of direct greenhouse-gas emissions modelling. Energy reduction is environmentally beneficial, but nitrous oxide produced by biological processes for nitrogen removal can be an important source of treatment related climate impact, and might respond non-linearly to DO and loading.

Future work should test the framework on multiple years of plant historian data, returning prediction intervals, and seeking to make the objective function more interesting by including carbon intensity, chemical dosing, sludge production and regulatory violation probability as targets. Hybrid physics-informed machine learning could improve generalizability by learning residual terms from activated-sludge mass-balance models, enabling comparisons against the present approach using reinforcement learning within the same control-theoretic constraints. Finally, digital-twin integration would allow stress-testing of control recommendations before implementation.

6. Conclusion

This study proposed an artificial intelligence-powered framework for optimisation of wastewater treatment by means of machine learning prediction and constrained process optimisation. Based on a 16,128-sample BSM1-inspired synthetic benchmark, the extreme gradient boosting algorithm outperformed multiple linear regression, random forest and Extra Trees regressors in simultaneous prediction of energy demand and effluent-quality indicators. The model demonstrated R^2 of 0.995 for specific energy, 0.970 for effluent TN, 0.987 for NH4-N and 0.981 for relative EQI. Combined with constrained particle swarm optimisation, the framework decreased the simulated specific energy demand by 22.5% and improved the combined effluent-quality index by 9.7% on average across unobserved operating scenarios. The most influential controllable variables were found to be DO set-point and SRT. These results provide a basis for the use of AI powered predictive and prescriptive analytics in operator oriented energy conscious wastewater treatment plants. The proposed framework should be calibrated and validated at a pilot or a full scale plant taking into account seasonal variations, an uncertainty analysis, safety, cyber-security and other limitations for successful adoption.

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