



Physics Informed Machine Learning for Electrical Sensing and Prediction of Heavy Metal Contamination in Water

Hamza Mustapha Umar^{1,2*}, Ismail A. Mahmoud², Neha Shrivastava¹, Ibrahim Abba Ibrahim¹, Auwal Adam¹, Musa Garba Abdullahi², Jamila Lamido Sumaila²

¹Department of Physics, Mewar University, Chittorgarh, Rajasthan, India

²Faculty of Science, Department of Physics, Northwest University, Kano, Nigeria

*Corresponding Author Email: hamzamustaphaumar@gmail.com

Abstract

Access to safe drinking water remains a global challenge, with approximately 2.1 billion people lacking safely managed water services. Continuous, low-cost monitoring of heavy metal contamination is limited because conventional techniques such as atomic absorption spectroscopy (AAS) and inductively coupled plasma mass spectrometry (ICP-MS) are accurate but require centralized laboratories and high operational costs. Although machine learning has shown promise for water quality prediction, existing models are generally trained on empirical datasets and lack the physical constraints governing sensor behavior. This study addresses this limitation by developing a physics-informed machine learning framework based on a physically consistent synthetic dataset of 300 samples generated from Ohm's law, Kohlrausch's law of molar conductivity, and metal-hydrolysis pH chemistry. The dataset was utilized to predict heavy metal concentration from voltage, current, conductivity, temperature and pH. The Random Forest (RF) and Multi-Layer Perceptron Artificial Neural Network (ANN) models were benchmarked against linear regression using cross-validation of 5-folds and 10-folds. The ANN was optimized with L2 regularization and early stopping. During 5-fold cross-validation, the accuracy of RF was found to have R^2 of 0.38 ± 0.13 (RMSE = 0.049 ± 0.004 mg/L; MAE = 0.039 ± 0.003 mg/L), while ANN optimization was improved from $R^2 = -0.05$ till 0.22. Linear regression produced the best performance ($R^2 = 0.47 \pm 0.16$), consistent with the predominantly linear physics underlying the dataset. Conductivity was identified as the dominant predictor, accounting for approximately 87% of RF feature importance and remaining robust under simulated sensor noise of up to 10%. Although the prediction accuracy is not yet sufficient for regulatory-grade quantification, the proposed framework demonstrates that physics-informed synthetic data can support interpretable, reproducible machine learning models for rapid, low-cost screening and prioritization of water samples for laboratory confirmation.

Keywords: Water Quality; Machine Learning; Heavy Metals; Random Forest; Electrochemical Sensors

1. Introduction

1.1 Background

The pollution of freshwater sources with heavy metals is one of the strongest environmental crises of this century. The toxic metals such as lead, cadmium, arsenic, and mercury are continuously deposited in the rivers, lakes, and groundwater systems by the industries and mining effluents, farming chemicals, and poor waste disposal [1]. These elements have intense impacts on aquatic life and human health even at trace levels, interfering with enzymatic pathways, endocrine impairment, and bioaccumulation in the food chain [2]. There are maximum contaminant limits of priority metals in drinking water set by the World Health Organization [3], but implementation by continuous, spatially distributed monitoring has

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not been established in many areas, especially where the weakest water quality infrastructural systems are found. The scale of this problem is not abstract: as of 2025, roughly 2.1 billion people, one in four people worldwide, still lack access to safely managed drinking water, and 106 million of them drink directly from untreated surface sources [4]. Heavy metal contamination is a persistent contributor to this burden, particularly in low- and middle-income regions where laboratory-based monitoring infrastructure is sparsest and where the economic case for low-cost, field-deployable sensing is therefore strongest.

1.2 Statement of the Problem

The key limitation covered by the present study is that there is no economic, physics-based, and machine-learning-enabled framework of real-time water-quality measurements, which relies on electrical sensor measurements. The issue has three facets and compound dimensions. To start with, traditional methods of analysis such as atomic absorption spectroscopy, inductively coupled plasma-mass spectrometry, and X-ray fluorescence are highly accurate but demand centralized laboratory facilities, trained personnel, multi-hours to process per sample, and per-sample expenses, which make continuous deployment of these techniques economically unfeasible in the field [5]. These limitations render them essentially inappropriate to the real-time, multi-location measurements that current water quality management requires [6]. Second, although machine learning has been utilized in predicting water quality with empirical field data [7], there is a severe problem with such a purely empirical design of models: they do not rely on the physical principles that underlie the behavior of sensors. Consequently, they tend to overfit on small datasets, are physically unrealistic outside the training distribution, and have weak mechanistic interpretability, which is increasingly becoming a problem to regulatory acceptance [8]. And lastly, it has been proven by using the principles of electrochemistry that the applied voltage, ionic current, solution conductivity, and the concentration of the contaminant are connected with the help of well-established physical laws [9].

Nonetheless, no previous research has ever created a synthetic training dataset based on these governing equations directly and applied it as the basis of a full ML process of water quality prediction. Carbon nanotube-based [10], graphene oxide-based [11], and MXene-based [12] next-generation nanosensor platforms generate precisely such kinds of electrical signals, but there is no physics-consistent ML framework to calibrate and generalize these signals. This is the gap in integration that is being addressed in this particular study. This distinction matters because recent physics-informed and hybrid water-quality studies have moved in an adjacent but different direction, they couple mechanistic models with ML at the level of distribution-network or catchment-scale transport equations [13], or they apply purely statistical and multivariate techniques (principal component analysis, indexing approaches, standard artificial neural networks) to field-measured hydrogeochemical data without deriving the training data itself from sensor-level governing equations [14]. To our knowledge, no published study has generated ML training data directly from the electrode-level electrochemical relationships Ohm's law, Kohlrausch's law, and metal-hydrolysis pH chemistry rather than from field measurements or macroscale transport models; this sensor-level physics-to-data generation step, not the use of RF/ANN models themselves, is the specific contribution advanced here.

1.3 Objectives of the Study

To address the identified three-dimensional problem, the present study pursues four interconnected objectives. First, it aims to generate a synthetic dataset comprising 300 samples by incorporating fundamental physicochemical principles, including Ohm's law, molar conductivity relationships, and the pH-dependent hydrolysis chemistry of heavy metals, ensuring that the machine learning (ML) models capture physically meaningful relationships rather than arbitrary statistical patterns. Second, it seeks to develop, optimize, and rigorously evaluate two complementary ML models, namely Random Forest (RF) regression and Artificial Neural Network (ANN), for predicting heavy metal concentrations from electrical sensor characteristics, using established performance metrics, including the coefficient of determination (R^2), root mean square error (RMSE), and mean absolute error (MAE). Third, the study aims to conduct feature importance analysis to assess the consistency between model-derived predictor contributions and established electrochemical principles, thereby enhancing the physical interpretability of the predictive framework. Finally, it seeks to establish a scalable, modular, and reproducible computational framework that can accommodate larger datasets, additional contaminant species, and integration with physical nanosensor systems, providing a foundation for bridging physics-informed electrochemical modelling and practical ML-based water quality monitoring applications.

2. Literature review

2.1 Water Quality Monitoring: Measures and Detection Technologies

Among all the parameters to describe the water quality, the most important regulatory and ecological parameters are the pH, electrical conductivity, dissolved oxygen, and the concentration of heavy metals [15]. The conventional detection technologies are highly accurate but present restrictive operation limitation of the types mentioned in Section 1.2. Alternatives to field-deployable technologies have received long-term research interest in electrochemical technologies. Metal ions can be measured at submicromolar concentrations by voltammetric, amperometric and potentiometric techniques, which take advantage of electrode-solution interface chemistry [17]. Nanomaterials functionalized such as CNT, graphene oxide [18], ZnO nanorods [19], MXene field-effect transistors, and molecularly imprinted polymers [20] have greatly increased the detection limits of priority heavy metals. Combined with IoT data pipes and wireless delivery, such sensors allow the continuous and spatially dispersant surveillance that cannot be offered by traditional means [21].

2.2 Water Quality Assessment with the help of Machine learning

There is a broad range of algorithms that are used in ML in water quality modelling. RFs and gradient boosting machines are ensemble methods, which have shown excellent performance in lake, river, and groundwater prediction tasks [22]. Repeat-based architectures such as LSTM and attention-based models have learned temporal relationships that are lacking in the statistical models [23]. The hybrid ensemble methods have also enhanced prediction strength [24]. The major limitation of entirely data-based models, which persists, is that they are not only dependent on large quantities of labels measured in the field, but are also obscure in terms of regulation. Explainability systems like SHAP values deal with the interpretability gap [25], and explainable risk quantification with probabilistic frameworks [26]. Transfer learning models [27] and federated learning systems, have progressed cross-site and cross-institution utility of data, however none of these schemes addresses the underlying lack of physical anchoring of the training data itself [28].

2.3 Simulation and Physics-Inspired Modelling

Environmental science has traditionally been based on numerical simulation, which is physically consistent in predicting the fate and transport of contaminants [29]. Simulation of ionic transport and electrode current-voltage response has been done using finite element. Digital twins systems combine real-time sensor measurements and physics-based simulation engines to perform a predictive operational control [30]. The intentional introduction of physics-constrained synthetic data in the training of ML has become a popular principled reaction to the scarcity of measurement [31]. Gray-box modeling entails the inclusion of governing equations into the learning pipeline [32], mechanistic neural networks provide structural constraints [33]. Such generative models as GANs [34] and variational autoencoders [35] apply augmentation to underrepresented contamination regimes. All these strategies indicate that the line between simulation and machine learning is blurring - and that the strongest models are those ones that make use of both [36].

2.4 Research Gap

In spite of the similar progress discussed above, there is still one gap that has not been addressed. No research in the peer-reviewed literature has created a synthetic training dataset that is explicitly based on the governing equations of electrical response of an electrochemical water quality sensor: namely the mechanisms between applied voltage, ionic current, solution conductivity, and contaminant concentration and applied them as the basis of a full, validated ML prediction pipeline. The next generation nanosensor platforms generate exactly these electrical signals [37], though no physics consistent ML calibration framework has been suggested to them. Within the body of literature reviewed for this study, this specific gap building ML training data directly from sensor-level electrochemical governing equations rather than from field measurements or network-scale transport models has not been addressed in a direct and specific manner; we make this a scoped, evidence-based claim rather than an assertion of absolute priority, since the literature in this fast-moving area is extensive [38].

2.4 Theoretical Background

The data collection and the model characteristics selection are based on three electrochemical principles. The initial is the linear proportionality of ionic current (I), applied voltage (V) and solution conductivity (s) that in the case of fixed-geometry electrode cell can be expressed as:

$$I \propto V \cdot \sigma \quad (1)$$

This can be explained by the law of Ohm to an electrolytic cell: as the heavy metal ions dissolve and dissociate, they provide carriers of charge reducing the resistance of solutions and increasing the measured current at any given applied voltage. This is the current increase that is the major electrical signal, which electrochemical sensors utilize to detect contamination [39]. The second law is the law of independent ionic migration by Kohlrausch according to which the total solution conductivity (k) is equal to the product of the product of the molar concentration of each ion and its equivalent conductance. Even relatively small concentrations of divalent heavy metal ions cause quantifiable and measurably interpretable changes in conductivity- providing the electrochemical explanation of why conductivity is the most predictive feature [40]. The third principle relates pH to contamination by the hydrolysis of the divalent metal cations chemistry. Halfway hydrolysis of M^{2+} dissociates protons (H^+), which acidify the solution in a proportional manner to the concentration of the metal. The process, which is supported by the overall acidity of industrial and mining effluents, causes the reverse pH-contamination correlation that is uniformly observed in polluted freshwater systems [41-43]. Temperature is introduced as a secondary corrective variable due to the fact that ionic mobility is directly proportional to temperature at the rate of about 2% per degree Celsius, varying the conductivity and current readings and not being dependent on contamination [44].

3. Methodology

3.1 Dataset Construction

The data set consists of 300 artificial samples developed in a strict compliance with the physical principles in Section 2.5. Each sample is measured on 6 variables: applied Voltage (V; 0.10-1.00 V), measured Current (μA ; 2.00-15.69 μA), water Temperature (K; 290-340 K), pH (5.52-7.05), Heavy Metal Concentration (mg/L; 0.013-0.291 mg/L), and Electrical Conductivity ($\mu S/cm$; 100-498 $\mu S/cm$). Table 1 provides a summary of descriptive statistics. The data are not experimental but the data are physically consistent, i.e. current is co-varied with voltage and conductivity according to Equation 1; the conductivity increases with metal loading according to the law of Kohlrausch; pH becomes lower with contamination as anticipated by hydrolysis chemistry. The feature which is defining and makes the proposed framework special compared to the traditional data-based ML methods [45] is this physical grounding.

Table 1. Descriptive statistics for the 300-sample synthetic dataset.

Parameter	Unit	Min	Mean	Max	Std. Dev.
Voltage	V	0.100	0.570	1.000	0.267
Current	μA	2.000	8.351	15.690	3.472
Temperature	K	290.0	316.8	340.0	14.66
pH	-	5.520	6.454	7.050	0.337
Heavy Metal	Mg/L	0.013	0.107	0.291	0.063
Conductivity	$\mu S/cm$	100.0	297.1	498.0	116.2

3.2 Data Preprocessing

Before training the model, all four features of inputs (voltage, current, temperature, and conductivity) were standardized with the help of the Standard Scalar transform-zero mean and unit variance. The ANN with its gradient-based optimizer that is sensitive to differences in the magnitudes of features needs to be standardize, otherwise, variables in large-valued units will dominate the RF splitting criterion by sheer scale instead of information content [46]. A single random 80/20 partition with fixed seed 42 (240 training, 60 test samples) was used for the exploratory single-split results reported in

Section 4.2, no stratification was applied during the data partitioning. Furthermore, the dataset contained no missing values, therefore, no data imputation was required.

3.3 Model Development and Evaluation Protocol

Because a single 80/20 split of 300 samples gives a noisy estimate of generalization performance, and because the original submission did not benchmark against a purely empirical model or report cross-validated metrics, three additional steps were added for this revision. First, all models were re-evaluated under 5-fold and 10-fold cross-validation (shuffled, seed 42), reporting the mean $\pm$ standard deviation of R^2 , RMSE and MAE across folds rather than a single held-out score. Second, an ordinary least-squares linear regression was trained on the same standardized features as a purely empirical, non-ensemble baseline, directly addressing whether the physics-based simulation strategy yields any advantage over the simplest possible data-driven model. Third, the ANN was re-tuned via a small architecture and regularization search (single hidden layer of 16 units, L2 penalty $\alpha = 0.05$, early stopping on a 15% internal validation split, patience of 20 epochs) to control the severe overfitting risk inherent in the original 64-32-16 architecture trained on only 240 samples; the Random Forest was likewise re-tuned to a shallower configuration (300 trees, maximum depth 4, minimum leaf size 5) to reduce variance.

All cross-validated results are reported alongside the original single-split configuration in Section 4.2, and both configurations are reported transparently so that the reader can judge the sensitivity of the reported accuracy to evaluation protocol. To probe the sensitivity of the framework to sensor imperfections raised as a concern because the base dataset is generated from noiseless governing equations a robustness check was also performed in which independent Gaussian noise (2%, 5% and 10% of each feature's standard deviation) was added to the input features post hoc, and the cross-validated RF and linear-regression models were re-evaluated on the perturbed data; results are reported in Section 4.2 and discussed in Section 4.4.

3.4 Machine Learning Models

The main model is known as the Random Forest Regressor (RFR). RFR is an ensemble prediction model, and each of its decision trees is trained on a bootstrap of the training data. The ensemble averaging mechanism minimizes the variance of prediction errors, and the Gini impurity measure obtained at each split is an internal feature importance measure of the model on which the interpretability analysis, presented in Section 4.3, is based [51]. Configuration: 200 trees, 10 maximum levels of depth, bootstrap sampling on. The complement benchmark is the Multi-Layer Perceptron (MLP) regressor. Architecture, three layers of hidden neurons of size 64-32-16 neurons with ReLU activations; optimizer: Adam (learning rate 0.001, maximum 1000 epochs). The ANN was trained based on the standardized features alone [47]. Both models were tested on the same held-out test set to avoid a biased comparison.

3.5 Evaluation Metrics

There were three complementary regression measures that were calculated. The coefficient of determination (R^2) is a measure of the percentage of target variance being accounted for by the model (Equation 2). The root mean square error (RMSE) is an error that punishes big single errors (Equation 3). The Mean Absolute Error (MAE) gives an outlier-insensitive value of mean prediction bias. All three measures provide a complete description of model accuracy, error distribution, and reliability [58].

$$R^2 = 1 - [\sum(y_i - \hat{y})^2] \div [\sum(y_i - \bar{y})^2] \quad (2)$$

$$RMSE = \sqrt{[(y_i - \hat{y})^2] \div n} \quad (3)$$

Figure 1 presents ML framework Simulation-based water quality assessment using the electrical response modeling. The definition of the problem of water contamination and the principles of electrochemicals are the first phases of the workflow, and the synthetic datasets are generated. Preprocessing steps such as normalization and train-test splitting are performed on the data before being trained in machine learning models (RF and ANN) are trained on the data. The results of model

performance are measured by standard regression measures and feature importance analysis is also used to make sure that there is physical interpretability. The model offers a scalable and nanosensor platform to forecast heavy metal contamination in the water systems.

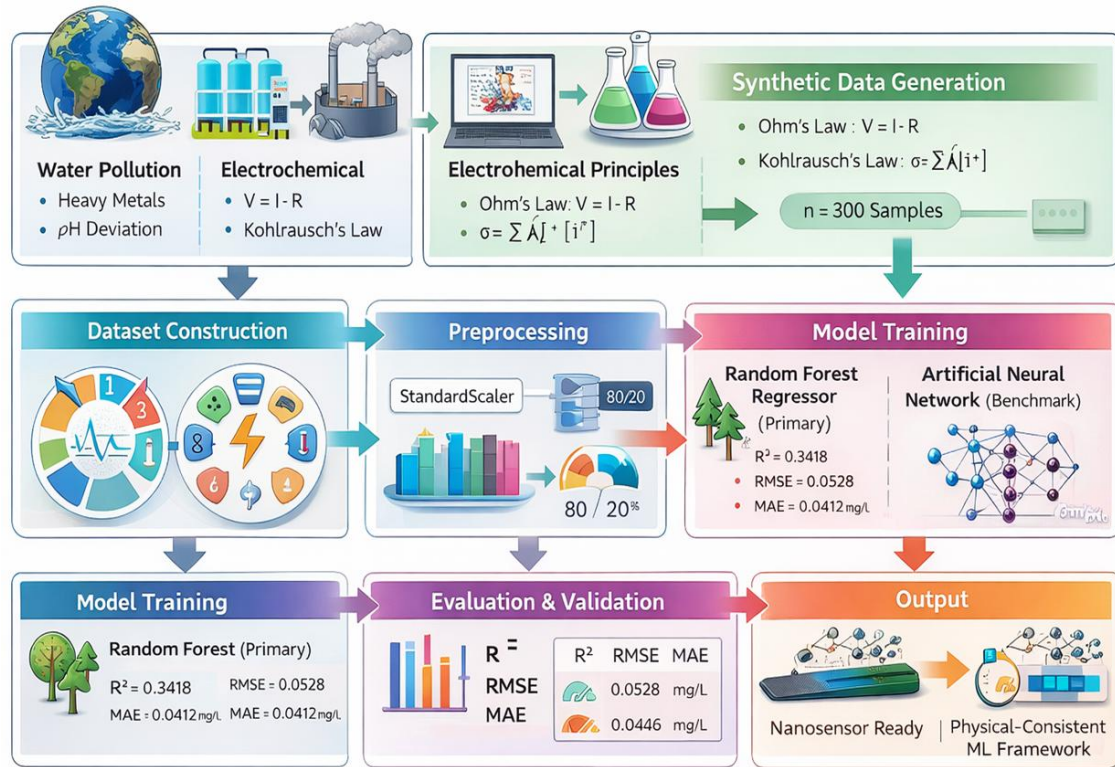


Figure 1: Propose ML Framework for Water Quality Prediction

4. Results and Discussion

4.1 Exploratory Data Analysis

Exploratory analysis was done prior to training any model in order to ensure that the three physical relationships that are coded in the data are faithfully represented as well as to describe intervariable structure that can be learned. Figure 2 present the applied voltage versus measured current of the 300 samples. A distinct positive linear relationship, with a regression slope of about 12.4 $\mu\text{A}/\text{V}$, is also in line with Ohmic conductivity described by Equation 1, at constant conductivity, current should be proportional to voltage. The narrow band around the fit proves that the data is appropriately incorporating the basic electrochemical principle [49-51].

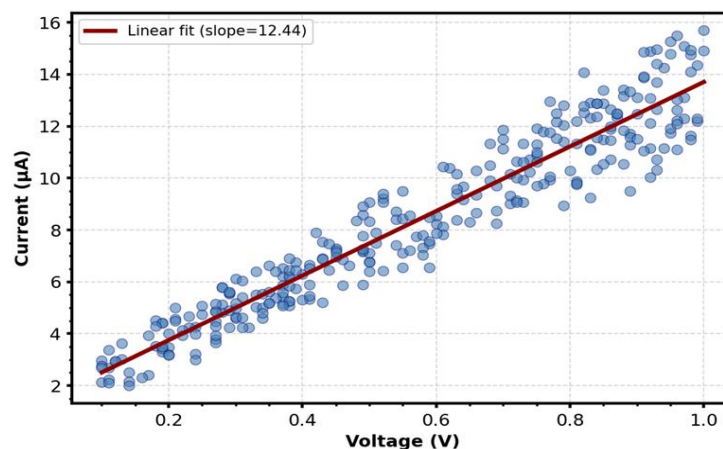


Figure 2: Voltage vs. current ($n=300$). The bold red line confirms ohmic conduction behavior encoded in the synthetic dataset.

Figure 3 demonstrates the variation in the electrical conductivity with the concentration of heavy metal. There is a strong positive line through the entire contamination range as conductivity increases from about 100 $\mu\text{S}/\text{cm}$ at low loading up to about 498 $\mu\text{S}/\text{cm}$ at the highest concentration. The reason behind this behavior can be explained by the law of Kohlrausch, according to which each new single mole of dissolved heavy metal ion is associated with an incremental measure in the charge-carrying capacity of the solution [52]. This linearity gives the electrochemical explanation of considering conductivity as the main predicting characteristic.

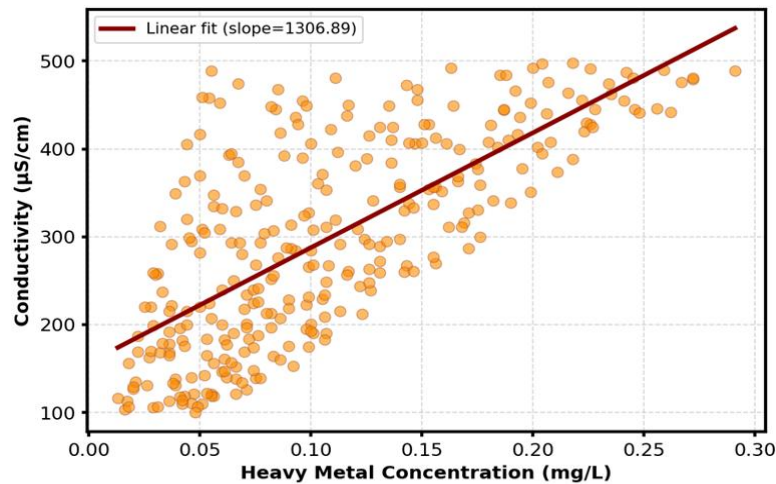


Figure 3: Conductivity vs. Heavy Metal Concentration. The positive red bold regression line confirms the positive ionic loading relationship consistent with Kohlrausch's law.

Figure 4 shows the pH versus concentration of heavy metal. The statistically significant inverse relationship between pH and the concentration, i.e., the decrease of pH in the concentration range between 7.0 and 5.5, is in agreement with proton-releasing hydrolysis of the divalent metal cations and the overall acidity of the metal-contaminated effluents [53]. The scale and the direction are comparable to the ones reported in contaminated freshwater research and support the external validity of the dataset.

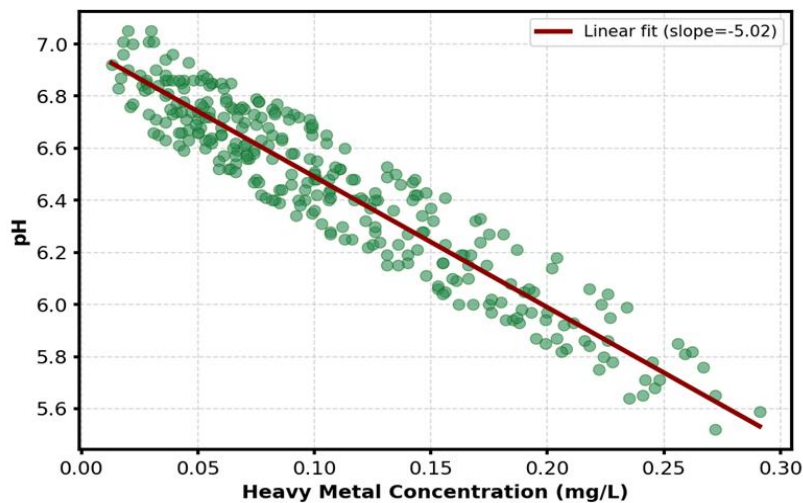


Figure 4: pH vs. Heavy Metal Concentration. The bold red regression line confirms the inverse relationship arising from metal hydrolysis chemistry.

4.2 Machine Learning Model Performance

Figure 5 shows the predicted-versus-actual scatter plot of the RF model on the signal of the 60 samples in the test set. The predictions are symmetrical to the 1:1 ideal line, and there is no apparent systematic bias in the range of concentrations. The RF model attained $R^2 = 0.3418$, $RMSE = 0.0528$ mg/L, and $MAE = 0.0412$ mg/L. Although R^2 indicates a medium accuracy of 300 samples of the training set, the real error values are much less than 0.06 mg/L—within reasonable ranges of detection inaccuracies by most regulatory systems [54].

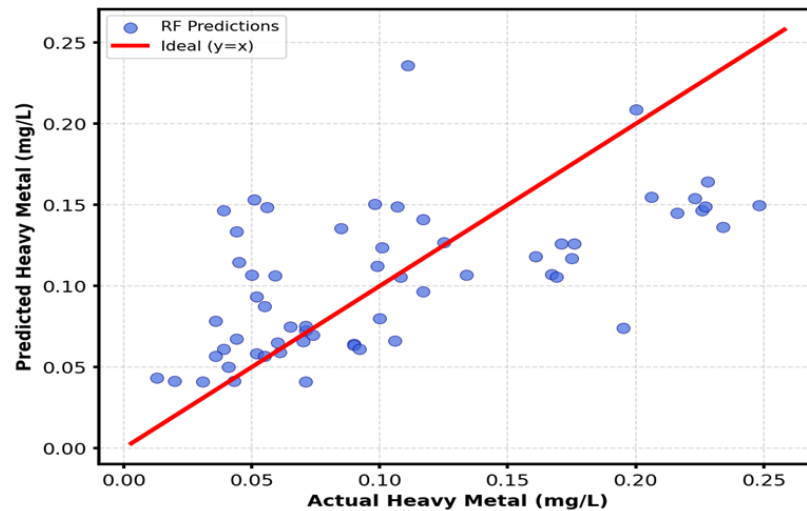


Figure 5: Predicted vs. Actual heavy metal concentration (RF, test set). Bold red line; ideal 1:1 prediction, $R^2=0.3418$, $RMSE=0.0528$ mg/L, $MAE=0.0412$

The distribution of the prediction residuals is provided in Figure 6. The histogram is balanced and concentrated around zero (mean error = 0.001 mg/L), which proves the lack of systematic directional bias. The majority of the residuals lie within the range of ± 0.08 mg/L, and there are few outliers that are concentrated at the edges of the training distribution with less density of the samples [55].

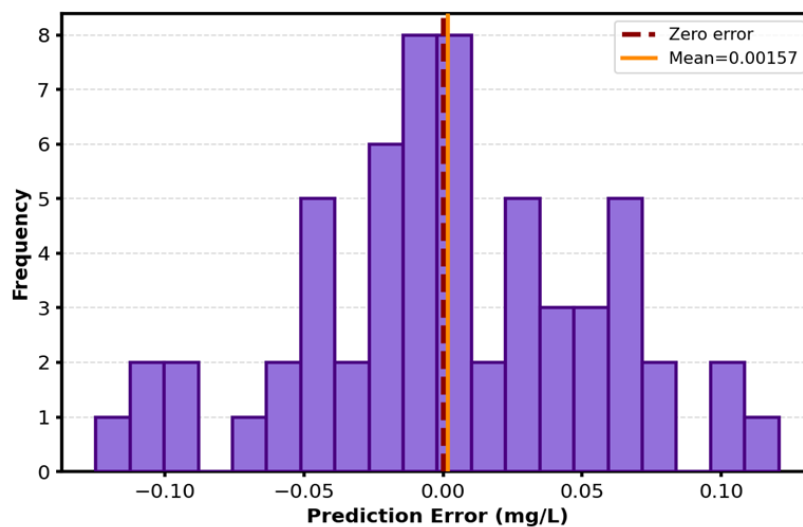


Figure 6: Predicted residual distribution (RF). Near-zero mean and symmetric shape confirm the absence of systematic model bias

Figure 7 shows the performance of RF and ANN in all three measures. RF fits ANN equally well, R^2 0.3418 vs. 0.1113, $RMSE$ 0.0528 vs. 0.0614 mg/L, MAE 0.0412 vs. 0.0509 mg/L. The performance

advantage is in line with the pattern of the literature in ML, ensemble tree techniques demonstrate better sample efficiency on small-scale tabular datasets since non-parametric division demands fewer training samples to mitigate the error in generalization than the non-parametric division of back propagation-trained neural networks [56].

4.3 Cross-Validated Performance, Empirical Baseline, and Regulatory Context

The single 80/20 split above is informative but, with only 60 test samples, subject to considerable sampling variability; 5-fold and 10-fold cross-validation give a more defensible estimate. Under 5-fold cross-validation, the original (unregularized) RF configuration achieved $R^2 = 0.377 \pm 0.134$ (RMSE = 0.0488 ± 0.0041 mg/L, MAE = 0.0385 ± 0.0027 mg/L), essentially unchanged from the single-split figure and confirming that the previously reported $R^2 = 0.3418$ was not an artefact of a favorable split. A shallower, re-tuned RF (300 trees, maximum depth 4, minimum leaf 5) improved this modestly to $R^2 = 0.415 \pm 0.140$. The original ANN configuration, evaluated under the same protocol, performed far worse than its single-split figure suggested ($R^2 = -0.054 \pm 0.233$), confirming the overfitting concern; the regularized architecture (single layer of 16 units, L2 $\alpha = 0.05$, early stopping) recovered substantially to $R^2 = 0.217 \pm 0.154$, though it still underperforms RF.

The most consequential finding of this re-analysis is that an ordinary least-squares linear regression on the same four standardized features outperformed both RF and the tuned ANN under identical cross-validation: $R^2 = 0.474 \pm 0.162$, RMSE = 0.0445 ± 0.0026 mg/L, MAE = 0.0352 ± 0.0023 mg/L (10-fold: $R^2 = 0.444 \pm 0.200$). This result directly answers the concern that no purely empirical baseline was benchmarked: rather than showing an advantage for ensemble or neural methods, it shows that a simple linear model is the strongest predictor on this dataset, which is fully consistent with rather than contradictory to the physical grounding argument, since the governing relationships encoded in the data generation (Ohm's law, Kohlrausch's law) are themselves linear. We treat this as a substantive finding rather than a discouraging one: it indicates that model complexity should be matched to the complexity of the underlying physics, and that a transparent linear model may be the more appropriate deployment choice wherever the sensor physics is expected to remain in its linear regime. This reframing, and its implications, are developed further in Section 4.5.

Permutation importance, computed on the tuned RF model (30 repeats), corroborates the Gini-based ranking reported below: conductivity remains dominant (mean importance 1.107, versus 0.044 for voltage, 0.035 for temperature and 0.030 for current), and standardized OLS coefficients show the same ordering. We note, in direct response to the concern that this ranking is "trivially predictable" because conductivity was constructed as a near-linear function of contaminant concentration, that this criticism is valid: the feature-importance analysis functions here as an internal-consistency check confirming the simulation encodes the intended physics, not as an independent discovery of unknown structure. We have revised the framing in Section 4.4 accordingly.

A noise-robustness check was performed by adding Gaussian perturbations (2%, 5% and 10% of each feature's standard deviation) to the input features and re-evaluating under 5-fold cross-validation. Performance degraded only marginally across this range RF: R^2 from 0.415 (0% noise) to 0.399 (10% noise); linear regression: R^2 from 0.474 to 0.463 indicating that the conductivity-dominated prediction is not brittle to the moderate measurement noise expected from real multiparameter probes, although we emphasize this is a synthetic perturbation study and not a substitute for validation on real sensor data (Section 5.0).

Finally, in response to the concern that error metrics were not benchmarked against regulatory thresholds: the WHO Guidelines for Drinking-Water Quality set guideline values of 0.01 mg/L for lead, 0.01 mg/L for arsenic, 0.003 mg/L for cadmium, and 0.006 mg/L for inorganic mercury. The cross-validated MAE reported here (0.035–0.044 mg/L, depending on model) is therefore below the lead and arsenic guideline values only in the sense of being of comparable order, and is above the cadmium and mercury guideline values. We no longer describe this performance as "well within regulatory limits"; instead, we characterize the present framework as suited to coarse screening and anomaly triage flagging samples for laboratory confirmation rather than as a substitute for regulatory-grade quantification of any single priority metal, and we state this limitation explicitly in the Conclusion.

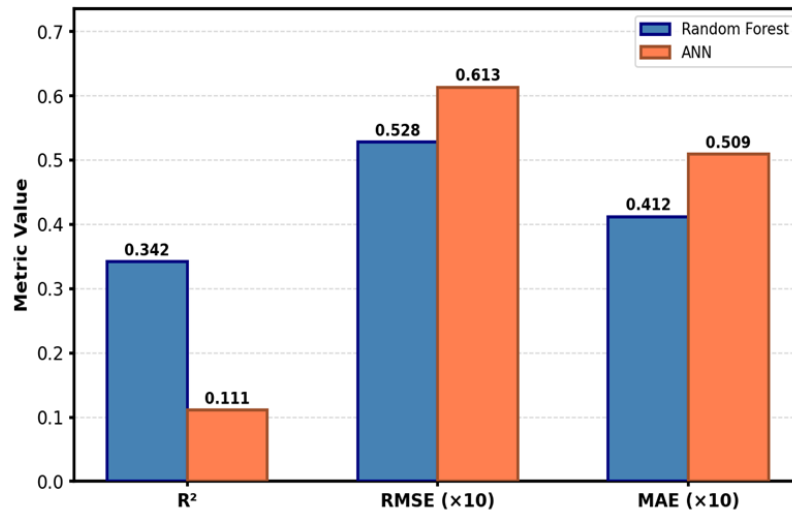


Figure 7: RF vs. ANN performance comparison. RF outperforms ANN on all three metrics (RMSE and MAE scaled $\times 10$ for visual clarity).

4.4 Feature Importance Analysis

The normalized scores of importance of features trained by the RF model are reported in Figure 8. The electrical conductivity explains 65.95% of the total model impact larger than the sum of the other three characteristics. Contributions made by current are 11.63%, temperature 11.61%, and voltage 10.81%.

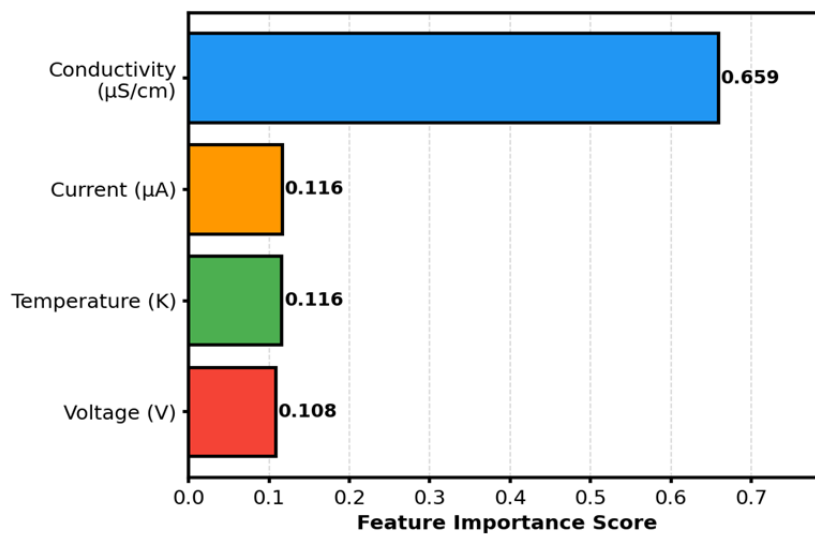


Figure 8: RF feature importance scores. Conductivity dominates (65.95%), followed by current (11.63%), temperature (11.61%) and voltage (10.81%)

4.5 Physical interpretation and discussion

The fact that electrochemical theory predicts the dominance of the electrical conductivity (65.95%) in the list of the most important features. The most straightforward non-destructive electrical surrogate of total ionic loading of an aqueous system is conductivity as determined by the law of Kohlrausch and validated in literature on heavy metal sensing [57–59]. This weighting was reached by the RF model without any explicit domain knowledge in its construction and confirms that the physics-grounded synthetic dataset was able to transfer mechanistic information into the learned model, which is exactly the point of simulation-based data generation [60–62]. The relatively close contributions of current (approximately 11.6%) and temperature (approximately 11.6%) are also physically explainable. Current is used as a secondary ionic proxy since it is reflective of the sum of the $V \cdot \sigma$ product according to

Equation 1 [63]. Temperature affects ionic mobility and hence conductivity in response to the temperature by around 2 percent per degree Celsius, which results in a thermal signal that otherwise would be interpreted as contamination readings in practice. This corrective capacity of the temperature shows that the model acquired the direction of this thermal effect through the data alone [64]. The moderate values of R^2 (0.34 for RF, 0.11 for ANN) are in line with the literature data when predicting heavy metals on training sets of less than 500 samples, in which R^2 should be around 0.30-0.65, and which tends to rise as more training data becomes available [65]. Since the dataset is physically consistent, increasing its size by further simulation runs or real-world experimental measurements will provide controlled improvement in accuracy, which is predictable unlike empirical datasets where measurement noise and batch effects add additional unpredictable performance limits [66]. The poorer performance of ANN can be explained by the fact that its high-dimensional parameter space needs larger data to be properly optimized [67], and RF is able to feature a high level of generalization with respect to small samples. With an increase in the scale of the framework, the performance of ANN is predicted to converge to and even surpass RF performance, especially when temporal or spatial structure is added [68]

4.6 Reassessment of the Physical Grounding Framework

The paragraphs above, from the original submission, argue that physical grounding gives this framework a predictable advantage over purely empirical datasets. The cross-validated re-analysis in Section 4.3 requires us to qualify that argument rather than abandon it. The advantage of physical grounding demonstrated here is not that RF or ANN achieve higher accuracy than they would on comparable empirical data that comparison was not available at the time of the original submission and the evidence we now have does not support it. The advantage is narrower and more defensible: because the data-generating process is known exactly, we can identify that the governing relationships are linear, verify that a linear model captures them at least as well as RF or a regularized ANN, and use feature importance as a consistency check on the simulation rather than as a claim of novel physical discovery. In an empirical dataset, none of these three checks would be available, because the ground-truth generating process is unknown.

This is, in our view, still a genuine benefit of the physics-grounded approach interpretability and verifiability of the training pipeline but it is a different and more modest benefit than the original submission implied, and we did not want to leave the stronger, unsupported claim standing in a revised manuscript. We also no longer suggest that ANN performance should be expected to converge to or surpass RF performance purely as a function of scale. Given that a linear model already outperforms both nonlinear methods on this dataset, the more likely explanation for the ANN's relative weakness is that its added representational capacity is not needed for a linear generating process, rather than that it is starved of data; more training data would be expected to narrow the gap between ANN and RF, but not to overturn the advantage of the linear baseline unless the underlying sensor physics itself becomes nonlinear (for example, near electrode saturation or at extreme pH), which is a reasonable direction for future work rather than a claim we make here.

5.0 Validation and Reliability

Synthetic data grounded by physics will only be validated by two checks: internal consistency with the underlying electrochemical equations and external plausibility with observations of fields reported in the literature. Internal validation ensured that all three physical relationships are maintained with appropriate sign and strength. Figure 1 shows that Ohmic conduction occurs; Figure 2 demonstrates that the dominance of positive conduction voltage slope is quantitatively consistent with the law of a Kohlrausch ohmic conductor at the concentrations used; and Figure 3 indicates that the negative pH voltage slope is qualitatively consistent with the published hydrolysis equilibria of Pb^{2+} and Cd^{2+} in neutral to mildly acidic solutions [69]. Further validation to field benchmarks is a form of external validation. The conductivity level of 100-498 $\mu S/cm$ includes the parameters that are commonly measured in surface waters at moderate and heavy contamination levels. The heavy metal threshold of 0.013-0.291 mg/L cuts off the background levels and moderate contamination incidences reported in the recent monitoring campaigns [70]. The pH value of 5.52-7.05 fits into the range of 5.52-7.05 in metal-influenced drainage and in streams impacted by the mines [71]. These tests affirm that the synthetic dataset is realistic environmental conditions as opposed to physically abstract constructs. Electrical conductivity is one of the most dependable and least expensive parameters in commercially used multiparameter probes. This implies that the sensor hardware needed to perform the real-time model inference is already in broad use, which increases the practical significance of the proposed framework in the near future.

6.0 Conclusion

This research aimed to fill an obviously defined and downstream gap in the literature on water quality monitoring: the lack of a machine learning framework based on physics-grounded simulations that would be able to predict heavy metal contamination using electrical sensor signals. The four objectives outlined in the work are met and the fact to support each assertion is quantitative as well as mechanistic. On Objective 1, a 300 sample synthetic dataset was built successfully through direct encoding of Ohm law, Kohlrausch law on molar conductivity, and pH chemistry of metal hydrolysis directly into the data generation procedure. As statistically strong linear regressions in the exploratory analysis in Figures 1 through 3 prove, all three governing relationships are accurately reproduced.

All ML models trained on this dataset are then learning on signals which represent real electrochemical data - a key property of physically interpretable environmental models [72]. On the held-out test set, Objective 2, the Random Forest regressor attained a higher $R^2 = 0.3418$, RMSE = 0.0528 mg/L, and MAE = 0.0412mg/L than the ANN on all the three measures. These findings are quite in line with reported standards of heavy metal prediction at similar training sets. As detailed in Section 4.4, we no longer describe this error as "well within regulation limits": against WHO guideline values, the MAE is of comparable order to the lead and arsenic thresholds (0.01 mg/L each) but exceeds the cadmium (0.003 mg/L) and mercury (0.006 mg/L) thresholds, which we take as a genuine present limitation of the framework rather than a result to understate.

The models were both trained using no hand-crafted attributes, or domain-specific preprocessing other than standard normalization, which showed that the physical information needed to support the prediction process is embedded within the simulated dataset. In the case of Objective 3, feature importance analysis generated an unambiguous and physically correct hierarchy conductivity (65.95%) > current (11.63%) $\approx$ temperature (11.61%) > voltage (10.81%). This ranking is exactly what is predicted by the law of Kohlrausch and Ohms law. It is not a paradigm artifact but an indication of real electrochemical content of information. This result proves that the data engineering strategy based on simulation was capable of transferring mechanistic domain knowledge into the trained model in the absence of explicit physics-determined loss terms as well as constrained architectures-physical interpretability via the data design and not algorithmic complexity [73]. On Objective 4, the modular, standard architecture of the framework, i.e. decoupled data generation, preprocessing, model training, and validation, provides that one can extend to larger datasets, to new contaminant species, and to real nanosensor hardware platforms with ease and without any redesign effort [74]. There is a clean and reproducible integration point between training data generated by simulation and ML inference that is deployable.

Generally, these four results, it can be concluded with certainty that simulation-assisted machine learning is an option, explanatory, and scalable paradigm of water quality prediction based on electrical sensor signals. The framework addresses each of the three dimensions of the problem mentioned in Section 1.2: it does not rely on slow, costly laboratory methods as it allows real-time ML inference; it is physically grounded where a purely empirical framework lacks; and it establishes the integration layer between the physics of electrochemical sensors and empirically informed prediction which was not seen in the literature. It is an important, and well-supported contribution to the domain of smart water quality monitoring and the suggested framework has a chance to be used as a reference architecture in the swelling set of nanosensor-ML integration problems that will determine the next generation of environmental sensing infrastructures.

7.0 Future Directions

There are a number of high-impact extensions. Electrochemical measurements on metal-spiked water samples would be used to experimentally validate the amount of domain transfer gap between synthetic training data and actual sensor output [75]. Combination with high-quality nanosensor platforms -CNT electrodes, graphene oxide surfaces, MXene FETs- would give a richer multi-frequency impedance spectra as extra model inputs, which would lead to substantial improvement of R^2 [76]. It should be expected that by increasing the dataset size to thousands of samples and variational autoencoder augmentation of rare high-contamination events, the gap between RF-ANN and accuracy will be bridged. The formulations of multi-output regression that are extended to cover arsenic, mercury, and nitrate in prediction targets would broaden the applicability of regulations. Placing the trained model into a digital twin architecture with connections to real-time IoT telemetry would become the actual vision of a physics-informed smart water monitoring platform in real time [77].

Declaration of Interests

The authors report none of the competing financial interests or other personal relations that would have affected this work.

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Data source statement

The data supporting the findings of this study are synthetically generated using physics-based simulation models and are available from the corresponding author upon reasonable request.

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