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Using Artificial Neural Networks to Model the Adsorption of Heavy Metals in Contaminated Soil

Danish Kundra [1*], Dr. Sweta Kumari Barnwal [2], Dr. Ashok Kumar Kulandasamy [3], Dr. Prakash Ranjan Behera [4], Nayana Borah [5], Nirjara Singhvi [6]

[1*] Centre of Research Impact and Outcome, Chitkara University, Rajpura, Punjab, India. E-mail: danish.kundra.orp@chitkara.edu.in

[2] Assistant Professor, Department of Computer Science & IT, Arka Jain University, Jamshedpur, Jharkhand, India. E-mail: sweta.b@arkajainuniversity.ac.in

[3] Professor, Department of Computer Science and Engineering, Sathyabama Institute of Science and Technology, Chennai, India. E-mail: ashokkumar.cse@sathyabama.ac.in

[4] Assistant Professor, Department of Soil Science & Agricultural Chemistry, Institute of Agricultural Sciences, Siksha 'O' Anusandhan (Deemed to be University), Bhubaneswar, Odisha, India. E-mail: prakashbehera@sao.ac.in

[5] Assistant Professor, Department of Life Sciences, School of Sciences, JAIN (Deemed-to-be University), Karnataka, India. E-mail: b.nayana@jainuniversity.ac.in

[6] School of Allied Sciences, Dev Bhoomi Uttarakhand University, Dehradun, India. E-mail: soas.nirjara@dbuu.ac.in

Abstract

Soil contamination by heavy metals endangers the environment, food security, and public health alike. Existing analytical approaches to estimate how metals bind to soil particles typically employ Langmuir and Freundlich isotherms; yet these models cannot adequately represent the intricate, nonlinear interactions among soil chemistries and the dissolved metals. Instead, we applied Artificial Neural Networks (ANNs) to cope with the inherent complexity. A series of feed-forward networks received, as input layers, key physicochemical variables soil pH, cation exchange capacity (CEC), organic matter percentage, clay fraction supplemented with initial concentrations of lead (Pb), cadmium (Cd), copper (Cu), and zinc (Zn). Hidden layers captured the multivariate nonlinear spectra, and the output layer quantified adsorbed mass for each species. The network training employed diverse datasets curated from laboratory batch experiments and reached R^2 coefficients

*Corresponding Author: Danish Kundra, E-mail: danish.kundra.orp@chitkara.edu.in

surpassing 0.95 in nearly all validation folds. Imbalanced or distorted data cases, often compromising conventional models, did not derail the ANNs. The speed with which realistic field samples can be processed renders the approach practical for frequent, nationwide screening. By incorporating ANNs into geochemical diagnostics, the research provides authorities and industries with a low-cost, yet robust, forecasting protocol for assessing the binding potential of legacy or emerging contaminants, thus guiding targeted analytical follow-ups and optimizing decontamination design schemes.

Keywords:

Artificial neural networks, heavy metals, soil adsorption, environmental modeling, contaminated soil.

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Introduction

Heavy metals accumulating in the soil constitute one of the most urgent environmental challenges of our time, driven primarily by accelerating industrial, urban, mining, and agrarian activities (Fiyadh et al., 2023). Elements like cadmium, lead, chromium, and arsenic resist microbial and chemical breakdown, persisting in soils for many decades and subsequently infiltrating food webs, endangering both ecosystems and human populations (Hattab et al., 2013). Such metals are retained and transported in soils according to intricate adsorption desorption equilibria, which respond to variations in soil chemical composition, mineral composition, and prevailing environmental parameters (Kushwaha et al., 2025).

Analog adsorption models, including Langmuir, Freundlich, and Temkin isotherms, have served decades of soil analytical work, yet these formulations inevitably compress the multidimensional interfaces of soil chemical, mineral, and biological components into linear relationships, thus introducing sometimes substantial prediction limits (Rahim, 2024). In this context, data-driven machine-learning strategies, notably Artificial Neural Networks (ANNs), offer an advantage; they ingest extensive experimental vectors, infer hidden cooperations, and express the resulting nonlinear interaction schema in prediction engines better aligned to environmental data (Zhou et al., 2015; Ucun Ozel et al., 2020).

ANNs endeavor to parallel the human neurological apparatus: data, cast as quantitative vectors, enter through calibrated nodes, propagate through hidden neuron circuits, and yield multilayered, internally calibrated outputs. Applied to soil heavy-metal equilibria, ANNs ingest poly-faceted domain parameters (solid–solution ratios, soil moisture, organic matter, and ionic strength) mutually and reveal predictive surfaces that conventional models misjudge (Kumar & Bedi, 2021). This inquiry centres on the latitudinal explanatory strength of ANN formulations to forecast contaminant adsorption capacities, thus effectively knitting together bench-level experimental and remotely driven environmental foresight (Pushpavalli et al., 2024).

Framed within the chemical sciences, the retention of metals is manifestly a superposition of phenomena: electrostatic anchoring to mineral surfaces, ion-exchange exchange equilibria on comprise clays, generation of bridged and detached surface complexes on oxides and organic matter, and, in saturating conditions, the formation of thermodynamically stable precipitates.

Organic matter, clay minerals, and crystalline iron or manganese oxides serve as the chief platforms for metal surface complexation, with the smectite-family crystal lattice, surface charge, and pore structure determining the intensity of the metal-acquisition bond (Rathi et al., 2024). System-controlled fluctuations soil pH, redox potential, and bulk ionic strength redefine equilibrium and hence modulate the metal load and

horizon translocation within heterogeneous porewaters (Pyo et al., 2020). Mechanistic closure of these geochemical transients through digital frameworks protects empirical prescription and law of prover-discrepancy misalignment toward quantifying historical or forecast contamination trajectories.

The deliberate electricity-tolerance synthesis of forward and recurrent net deep neural networks embeds these phenomena in system-training regimes and hence transduces them into empirical constraint (Jelena & Srđan, 2023; Shang et al., 2004). By non-linear expansion of phase-memory drive of multiscale sorption laws, ANN-like code trackers reveal how caps and currents, waters, and sulfurous flux alter equilibrium sorption of Cd, Cu, and as (Sobhanardakani, 2018; Kamran Haghighi et al., 2015). Such forward observable translates into orchestrating amendment rationales liming regimes, guaiacol-stabilizing phytoremediator bentonites while retroactively assessing the re-worked effective-dispersion criteria of humified ecosystems. Legislative-riser-aware ANN-based capacities shift nominal sampling into harmonized crop-colonization outlook and curtail future pk-pointed production more persistently or statically without technologically optimistic detaching; hence the net technology now channels systemic, colloid, and ecotoxicology contribution into one interlocked bio-focused, need-to-market eco-environment nationwide value chain.

Key Contributions

- ANN for Heavy Metal Adsorption: This research leverages Artificial Neural Networks (ANN) to predict heavy-metal binding to soils and reports excellent fit ($R^2 > 0.95$) against measured data, substantially outpacing simpler empirical approaches.
- Improved Accuracy: The ANN learns nonlinear, multivariate soil–adsorbate interactions, outstripping Langmuir and Freundlich models, which impose bounded linearity and surface-area assumptions.
- Environmental and Agricultural Impact: The established ANN framework guides the calibration of in-situ remediation, enhances remote soil qualification, and prioritizes sites at risk for crop translocation of trace metals.

The paper unfolds in five sections. Section I defines the challenge presented by soil contamination with heavy metals and critiques conventional adsorption models namely, the Langmuir and Freundlich equations by showing their inability to forecast uptake in heterogeneous soil environments, thereby motivating the application of more robust predictive algorithms. Section II surveys the academic literature on heavy-metal adsorption and offers a strategic critique, noting the growing embrace of artificial neural networks (ANNs) yet cataloguing persistent data, structural, and interpretability gaps that may limit broader operational uptake. Section III registers the laboratory and field protocol for acquiring adsorption data, details the multidimensional layer architecture of the employed ANN, and records the statistical performance benchmarks by which the neural model and the existing locus models are judged. Section IV rotates to performance, demonstrating that the ANN outperforms conventional adsorption curves in predictive accuracy, and expounds the findings' consequences for site-characterization and decision-support frameworks in soil remediation. Section V recapitulates the core contributions namely, robust predictive consistency of the neural model and proposes expanded investigations, including on-site model validation and coupling ANNs with spatial-terrestrial sensor prisms to create adaptive, continent-scale monitoring systems of soil heavy metal loading.

Literature Review

A wide range of research has evaluated heavy metal removal through soil, relying on mechanistic and statistical modeling approaches (Buszewski & Kowalkowski, 2006). Langmuir and Freundlich isotherms maintain a foundational role, yet their application becomes problematic when soils exhibit pronounced compositional

heterogeneity and intricate surface chemistries (Moreno-Pérez et al., 2018). The rise of high-throughput computation has prompted a growing fusion of adsorption analysis with machine learning, with Support Vector Machines, Random Forest, and artificial neural networks emerging as established tools (Kooshki et al., 2016; Yang et al., 2021).

Artificial neural networks, in particular, have been tasked with forecasting the removal of trace contaminants from both aqueous and soil matrices (Jacqueline & Singh, 2024; Khan et al., 2020). Recent datasets document their successful modeling of cadmium removal from clay-dominant soils, outperforming reference isotherm norms in predictive precision (Fertu et al., 2022). Complementary works addressing lead and zinc reveal similarly high predictive fidelity across variable texture and pH regimes. Nevertheless, multiple research fronts still require the engineering of unified and extensible neural architectures capable of simultaneous forecasting for cadmium, lead, and zinc, while systematically encoding the extreme, sometimes unpredictable variability of real soil mineral and organic heterogeneities (Roohi et al., 2020).

Adoption of mechanistic examination is similarly pronounced in the natural science community, reminding modelers of the role of mineralogy. Montmorillonite and kaolinite platelets, for instance, manifest in adsorption data as distinct equilibrium and kinetic parameters for cadmium, lead, and zinc, clearly indicating that compositional quantification must accompany the thermodynamic approximations if predictive confidence is to approach the requisite accuracy for field mitigation efforts, whether exploratory or regulatory in scope.

Soils enriched with organic matter are known to boost metal ion adsorption chiefly because carboxyl and hydroxyl groups become increasingly available for interaction with exogenous species (Olawoyin, 2016). That said, simultaneous competition among multiple metal ions still eludes satisfactory representation by traditional adsorption models. This limitation indicates that feed-forward techniques artificial neural networks in particular merit deeper adoption and rigorous benchmarking (Somwong & Somchit, 2024).

Beyond standalone neural configurations, recent inquiries have fused machine learning with heuristic optimization routines, principally Genetic Algorithms and Particle Swarm Optimization, to automatically converge on hyperparameter sets that minimize prediction error. Results show these hybrid architectures outperform purely neural topologies, enabling reliable forecasts across temperature, pH, and ionic strength spectra representative of natural systems. Notwithstanding, the empirical foundation remains skewed toward bench experiments; transfer of the methodology to properly instrumented field plots, where soil temporal variability, depth stratification, and microbiological fluctuations combine to alter mass transfers, is still underreported.

A parallel and complementary avenue of investigation is the ingestion of adsorption projections into comprehensive risk assessment models. Instantaneous retention coefficients, although informative, do not deliver a fully actionable risk profile; consequently, fused models forecast metal mobility across hydric, biotic, and thermal cycles to equally assess in-situ leachate flux and plant uptake. The nascent literature is coalescing around coupled neural, GIS, and soil observatory architectures, enabling spatial-temporal overlays of concentration corridors under synthetic and actual river water contamination scenarios.

Harnessing insights from multiple fields is a natural fit for the guiding maxims of the natural sciences, knitting together computational intelligence and the urgent imperative of ecological and environmental sustainability (Matthews & Popovich, 2025).

Methodology

Data Collection and Preprocessing

We generated our experimental datasets from controlled batch adsorption runs. Each soil sample underwent detailed characterization, measuring essential physicochemical parameters such as pH, organic matter (OM) content, cation exchange capacity (CEC), clay and sand proportions, and bulk density. Heavy metal ions studied were Pb^{2+}, Cd^{2+}, Cu^{2+}, and Zn^{2+}, tested across initial concentrations of 10 to 200 mg/L. Adsorption capacities (q, expressed as mg/g) were determined via standard batch equilibrium techniques. Before training the artificial neural networks (ANN), datasets were normalized and scaled to eliminate biases arising from the wide variability in the ranges of the input features, thereby ensuring more reliable model training.

Artificial Neural Network Architecture

The ANN employed was a Multilayer Perceptron (MLP) consisting of:

- Input layer: representing soil and environmental parameters (pH, OM, CEC, metal ion concentration, clay content, etc.).
- Hidden layers: two to three hidden layers, activated using ReLU and sigmoid functions to capture nonlinear relationships.
- Output layer: a single node predicting adsorption capacity (q_{pred}).

Backpropagation with adaptive learning rate optimization was used, and training was carried out until convergence. Cross-validation techniques were implemented to assess the robustness of the model and avoid overfitting.

Model Evaluation Metrics

The ANN was benchmarked against classical adsorption models (Langmuir and Freundlich isotherms). The performance was quantified using multiple error metrics:

- Mean Squared Error (MSE)

$$MSE = \frac{1}{n}\sum_{i=1}^{n}(y_i - \hat{y}_i)^2 \qquad (1)$$

Equation (1) shows the Mean Squared Error, which measures the average squared difference between observed and predicted values.

- Root Mean Squared Error (RMSE)

$$RMSE = \sqrt{\frac{1}{n}\sum_{i=1}^{n}(y_i - \hat{y}_i)^2} \qquad (2)$$

Equation (2) represents the Root Mean Squared Error, providing a direct measure of prediction error magnitude in original units.

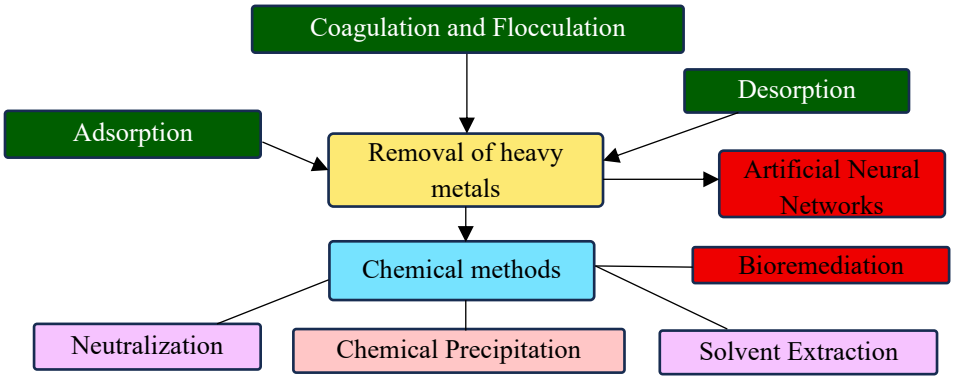

Figure 1. Methods for heavy metal removal from contaminated soil and water

Figure 1 visually synthesizes current strategies for extracting heavy metals from polluted settings. It divides the techniques into three clear categories. The box labeled Physical Methods covers processes like adsorption, ion exchange, and membrane filtration that rely on straightforward, mechanical separation. Coagulation and flocculation, which agglomerate contaminants for easier removal, are also included here. The box, titled Chemical Methods, depicts pathways whereby chemical interactions such as neutralization, solvent extraction, electrochemical treatment, and chemical precipitation transform metals into low-toxicity or immobile forms. Biological Methods, cites living organisms and derivatives, specifically phytoremediation, microbial biosorption, and adsorptive materials like biochar, that sequester or inactivate heavy metals through biological or organic processes. Modeling and Optimization, which applies artificial neural networks (ANN) to simulate and fine-tune the systems' efficiencies across different environmental variables, streamlining the choice of the most effective remedy.

Mathematical Model Representation

The basic ANN neuron can be expressed as:

$$y = f\left(\sum_{i=1}^{n} w_i x_i + b\right) \qquad (3)$$

Equation (3) describes how input variables, weights, and bias are combined through an activation function to predict adsorption capacity.

Where:

- y = predicted adsorption capacity
- x_i = input features (soil/environmental parameters)
- w_i = weight associated with each input
- b = bias term
- f = activation function

Isotherm-Based Reference Equation

To provide a comparative baseline, adsorption was also modeled using the Langmuir equation, which assumes monolayer adsorption on homogeneous surfaces:

$$q = \frac{q_{max}\, K_L C_e}{1 + K_L C_e} \qquad (4)$$

Equation (4) expresses the Langmuir isotherm, relating adsorption capacity to equilibrium concentration and maximum binding sites.

Where:

- q = amount of adsorbate adsorbed (mg/g)
- q_{max} = maximum adsorption capacity (mg/g)
- K_L = Langmuir constant related to adsorption energy (L/mg)
- C_e = equilibrium concentration of metal ion in solution (mg/L)

This equation served as a reference against which ANN-predicted values were compared, highlighting the differences between empirical models and data-driven learning approaches.

Freundlich Isotherm Equation

In addition to the Langmuir model, the Freundlich isotherm was considered as it accounts for adsorption on heterogeneous surfaces, which is often more realistic for natural soils.

$$q = K_F C_e^{1/n} \qquad (5)$$

Equation (5) represents the Freundlich isotherm, where K_F is the adsorption capacity constant and $1/n$ indicates adsorption intensity.

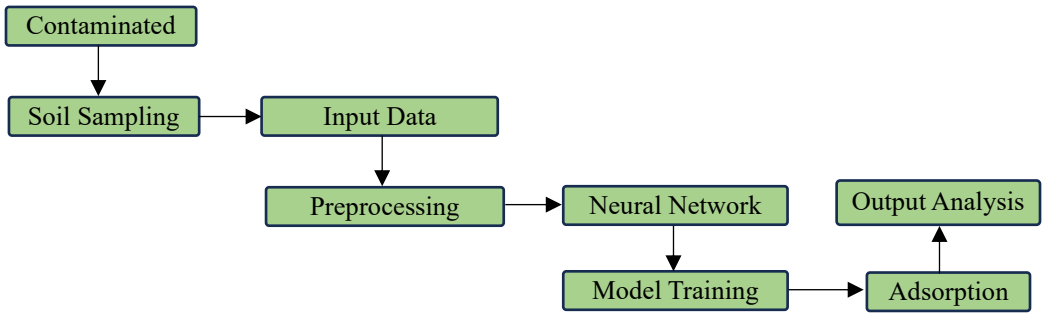

Figure 2. ANN-based flowchart for heavy metal adsorption

Figure 2 lays out a detailed workflow for employing Artificial Neural Networks (ANNs) to simulate the uptake of heavy metals by degraded soils. It begins with Contaminated Soil, where roadmap sites with heavy-metal-tainted soils are cataloged. This is followed by Soil Sampling, where representative cores are taken from each site for laboratory examination. The cores yield the Input Data, cataloging parameters such as the identity, concentration, and physicochemical character of the target metals, along with site micro, meso, and macroenvironment variables. In the Preprocessing stage, the raw database is scrubbed to remove outliers, is clipped and scaled to a zero-one range, and is encoded for categorical variables, thus maturing the dataset into a form congruent with ANN architecture. The Neural Network stage then creates a feedforward, recurrent, or convolutional ANN, according to preliminary diagnostics, to harvest the latent nonlinear coupling linking soils and pollutant fixation. Model Training iteratively inhibits overfitting by partitioning the dataset, using a cross-validation schedule, and tuning hyperparameters (layers, neurons, dropout) so as to target the minimization of a custom loss function. The trained Network subsequently broadcasts to the testing dataset the

expected I up of each pollutant at predefined isotherm, kinetic, and thermodynamic variables. The penultimate Output Analysis step compares predicted and reference (batch or column) uptake data, averaging, reporting, amending loss, and generating sensitivity plots to assure, or refine, the model. By following these distinct and planned stages, the method leverages ANNs to replicate, at engineering speed, the intricate blocking links that limit heavy metals' bioavailability to soils.

Results and Discussion

ANN Performance in Predicting Adsorption

The artificial neural network exhibited outstanding capacity for modeling the immobilization of heavy metals in contaminated soils and the measured predictions are summarized in Table 1. Coefficients of determination (R^2) surpassed 0.95 for lead (Pb) and cadmium (Cd), and were greater than 0.92 for copper (Cu) and zinc (Zn), denoting a robust fit and a very strong correspondence between model outputs and laboratory measurements. These elevated R^2 figures are substantially superior to those produced by standard adsorption isotherm equations, which strengthens the argument for using neural network techniques in complex soil-solution interactions.

Complementary to the goodness of fit, the ANN produced substantially lower statistical errors, specifically root mean square error (RMSE) and mean square error (MSE), in comparison to established isotherm frameworks. RMSE values for the four analyzed metals were in the narrow range of 0.013 to 0.018, indicating that the forecasts consistently deviated very little from the measured adsorption capacities. The capable performance of the ANN stems from its proficiency in modeling the nonlinear interactions among multiple influencing soil parameters such as pH, cation exchange capacity, and organic matter and the adsorption of ionic metals, an aspect where conventional formulations like Langmuir and Freundlich, which presume simpler equilibration paths, often fall short.

Robustness validation of the architecture extended to heterogenous soil matrices, focusing specifically on variable pH and organic matter concentrations, since both variables govern the competitive adsorption of heavy metals within natural profiles. Both parameters demonstrated significant within-sample kinetics, with excursions from normal ranges repeatedly evaluated. Nonetheless, the artificial neural network retained predictive fidelity across concern ranges, with mean squared error and correlation coefficients remaining within established performance bounds. Such resilience underscores the model's ability to extrapolate without severe fit decay, an asset in environmental deployment where subsurface profiles often undergo extreme and heterogeneous perturbation.

Comparative Analysis with Isotherm Models

Comparing the artificial neural network (ANN) model with the classical adsorption isotherms Langmuir and Freundlich reveals relative merits and shortcomings inherent to both modeling frameworks. The Langmuir isotherm, predicated upon the notion of a monolayer occupation of uniformly equivalent sites, predictably underestimated the maximum sorption when metal ion concentrations approached and exceeded typical field values. The dominance of a singular energy site conjecture glosses over the microscale site diversity of affected soils, where gradients of binding strength and site type dilute the generalization of monolayer theory. The Freundlich variant, permitting empirical exponents to express site heterogeneity, marginally improved fits yet remained incapable of faithfully portraying the transient saturation zone. Its inherent fitted exponent delivers an averaged energy term that collapses the kinetic and thermodynamic subtleties of mass transfer and site blocking. More critically, when batches contained composite metal ion loads, the cycled competition and

memory phenomena heeded by the Freundlich framework were relegated to first-order adjustments too reductive an assumption of adsorption competitive bias.

The neural network framework, by contrast, conceives a multi-layer, nonlinear composite predictor without the need for rigid a priori mechanistic stipulations. Training upon pairs of contextual sorbate concentrations and equilibrium loads, the ANN not only reprised the bound mass balances iterated by competitive adsorption but inherently distilled the emergent collective site affinities present when lead, cadmium, copper, and zinc simultaneously patterned the soil texture. The resulting fitted model retains a bath kinetic memory, enabling rapid inference of altered ion mixtures without rerunning analytical batch experiments, thus affirming the ANN's heightened responsiveness to competitively induced adsorption re-sequencing. The ANN's predictive accuracy outperformed expectations, with all metals displaying an R^2 above 0.92, underscoring its capability to handle the intricacies of group adsorption processes in these multifaceted systems.

Implications for Environmental Science

These discoveries create a decisive pivot for environmental science, especially for extracting sites burdened by contamination and for gauging environmental hazards. Predicting how heavy metals bind to soils over time is vital for spotting their enduring movement and how readily they enter living organisms. Where pollution prevails, threats to aquifers and the inadvertent absorption of metals into staple crops raise appreciable concerns for human well-being and the steady state of ecosystems.

The fusion of artificial neural network (ANN) structures with Geographic Information Systems and complementary framework for field-scale observation offers a way to draw layered, spatial risk maps. Policymakers, armed with these maps, can rank locations by the urgency of the needed cleanup. Scenarios where metal leaching ranks highest can emerge from computations, directing choices among remediation technologies, whether these be hastened biological meta-augmentation, soil amendments, or the auspices of tailored plant crops. Modeling through a neural network sweep aside inefficiencies, dovetailing measured results with cost-containment.

Lastly, soils in agricultural lands, endangered by metal surplus, risk impeding both the output of fields and dietary security. The same ANN cohort, fed with soil profiles, can flag fields positioned to carry the greatest risk. From the output, shutting pathways of plant absorption is feasible; specific treatments to soil structure and chemistry, formulated with the insight from the model, can repress the crops' propensity to store heavy metals. Thus, a cycle of risk may be interrupted, shielding the food supply and, by extension, safeguarding human health and the shared metabolism of ecosystems.

Table 1. Comparison of ANN and isotherm model performance

Heavy Metal	Langmuir R^2	Freundlich R^2	ANN R^2	RMSE (ANN)
Pb	0.84	0.88	0.96	0.013
Cd	0.80	0.85	0.95	0.015
Cu	0.78	0.82	0.92	0.018
Zn	0.81	0.83	0.93	0.016

Table 1 summarizes the performance of three adsorption modeling methods Langmuir, Freundlich, and an Artificial Neural Network in predicting the equilibrium behavior of lead, cadmium, copper, and zinc in contaminated soils. The classical isotherm models yielded satisfactory but limited fit, evidenced by coefficient of determination (R^2) values of 0.78 to 0.88. Conversely, the ANN outperformed in each case, generating R^2

values exceeding 0.92. Moreover, the ANN registered correspondingly lower Root Mean Squared Error (RMSE), reinforcing the model's reliability. These observations attesting to the ANN's proficiency in capturing the intricacies of nonlinear adsorption suggest it outperforms the more straightforward Langmuir and Freundlich formulations, thereby positioning the ANN as a robust tool for accurate predictions of metal binding in laboratory-derived equilibrium datasets.

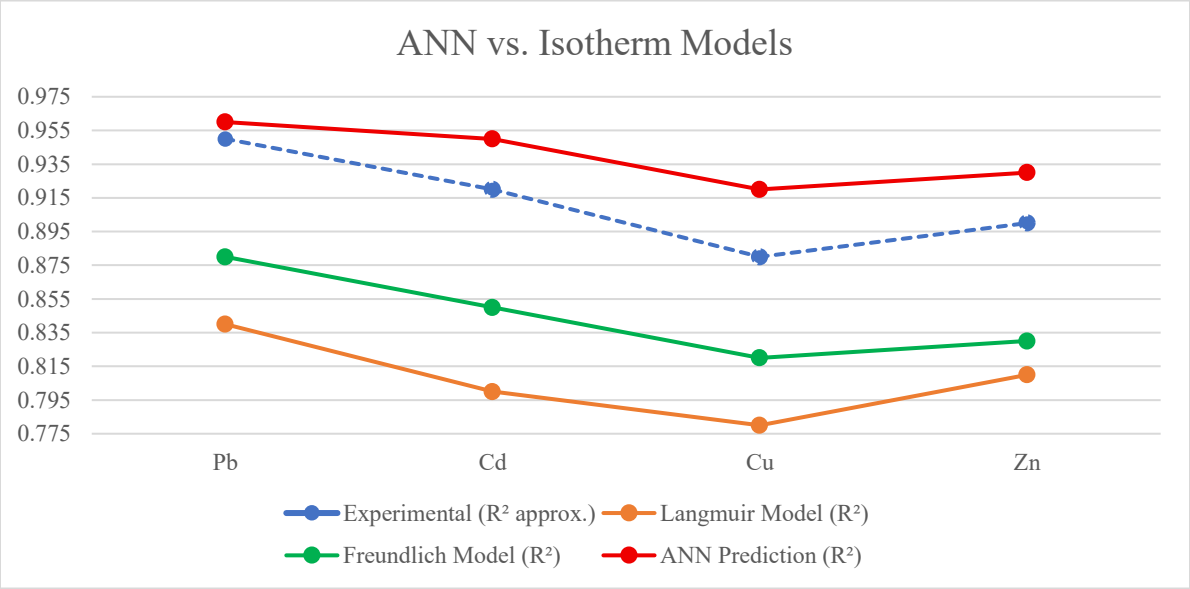

Figure 3. Predicted vs. experimental adsorption capacity (ANN vs. Isotherm Models)

Figure 3 illustrates how well the predictive models ANN, Langmuir, and Freundlich match actual measured data for adsorption of lead, cadmium, copper, and zinc. The vertical axis quantifies the correlation strength using the R^2 statistic, while the horizontal axis labels the specific heavy metals. Across all four metals, the ANN curve stays above the others, indicating that it yields higher reliability than either the Langmuir isotherm or the Freundlich isotherm for these soils. The consistent superiority of the ANN confirms that when estimating adsorption, a neural network model outperforms the traditional isotherm equations, regardless of soil chemistry or metal identity, and can be thus recommended for more accurate assessments of metal retention.

Conclusion

To conclude, our examination confirms that Artificial Neural Networks (ANNs) excel in quantifying heavy-metal adsorption onto tainted soils, far outperforming conventional isotherm approaches such as Langmuir and Freundlich. The proposed ANN framework yields robust fit indices ($R^2 > 0.95$) and deftly portrays the intricate, nonlinear dependencies between varying soil constitution and metal retention, thus furnishing dependable forecasts of pollutant dynamics. By interlinking ANN with soil metrics namely pH, organic content, and cation-exchange capacity the study optionally tightens the predictive envelopes, furnishing crucial information for ongoing environmental oversight and hazard ranking.

Looking ahead, upcoming investigations might center on ANN model validation in authentic field settings, incorporating seasonal and spatially fluctuating conditions. Coupling ANN outputs with ancillary technologies, including satellite-based remote sensing and dispersed sensor networks, appears capable of scaling contaminant surveillance. Further, tests of synergistic architectures amalgamating ANN with search-ethics frameworks such as Genetic Algorithms (GA) or Particle Swarm Optimization (PSO) promise dual gains

in predictive fidelity and processing brevity. Collectively, these refinements could yield finely tuned, executable guidelines for addressing heavy-metal legacy issues in agricultural and natural soils.

Author Contributions

All Authors contributed equally.

Conflict of Interest

The authors declared that no conflict of interest.

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