

Predictive modeling of metal recovery efficiencies from spent lithium-ion batteries using RSM enhanced residual neural network framework

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ABSTRACT

The increasing consumption of lithium-ion batteries (LIBs) has created a growing need for efficient recycling processes to recover valuable metals such as lithium (Li) and cobalt (Co). The present study analyses the performance of supervised machine learning models in predicting the leaching efficiencies of Li and Co from spent LIBs in the ultrasound-assisted leaching of Lithium Cobalt Oxide (LCO) cathode material using a Hybrid MW-US high-pressure chemical reactor. The standalone linear regression (LR), quadratic polynomial regression (QPR), neural network (NN) and random forest (RF) models were firstly evaluated by their ability to capture the relationship between key process parameters and the metal recovery efficiencies. Among the standalone models, the RF model demonstrated the strongest predictive performance. However, these purely data-driven models do not explicitly incorporate the empirical process relationships identified from the experimental leaching process. To address this limitation, an RSM-enhanced residual neural network (RSM-NN) framework was developed by integrating the response surface model (RSM) formulation from the original experimental study as an empirical process constraint during training. The proposed RSM-NN framework achieved very high predictive accuracy and produced smooth and consistent trends in the partial dependency analysis, reflecting the strength of the hybrid modeling framework. The results demonstrate the potential of RSM-enhanced machine learning frameworks for improved modelling and optimization of hydrometallurgical recovery processes from spent LIBs under the investigated experimental conditions.

1. Introduction

Lithium-ion batteries (LIBs) have attracted considerable attention in recent years due to their widespread use in portable electronics, electric vehicles, and energy storage systems. The rapid expansion of these technologies has led to a significant increase in the production and consumption of LIBs. This increased consumption results in a growing volume of spent LIBs being discarded at the end of their service life, posing an environmental challenge. Spent LIBs consists of a notable concentration of critical metals such as Lithium (Li), Cobalt (Co), Nickel (Ni), even in their discarded state [1]. Efficient recovery of these metals can contribute to resource conservation and sustainable materials management. In particular, the lithium cobalt oxide (LCO) cathode material in spent LIBs is an important source of Li and Co, and has been

widely studied in battery recycling research [2,3]. Among various recycling approaches, ultrasound assisted leaching process has been widely investigated for its improved ability to selectively recover valuable metals from spent LIBs [4,5]. It should be noted that the efficiency of the leaching process depends strongly on various operating process parameters such as temperature, reaction time and ultrasound power [6, 7]. Therefore, the development of predictive analytical models capable of investigating the relationship between the process parameters and metal recovery efficiency could provide valuable insights for process optimization and improved resource recovery from the spent LIBs.

Recent advances in recycling spent LIBs have focused on improving both the efficiency and sustainability of metal recovery processes. Ultrasound-assisted methods, including ozone-based systems and microbial leaching, have enabled high lithium extraction and in-situ

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separation of cathode materials from used LIBs [8,9]. Additionally, organic acids such as oxalic and citric acid, combined with ultrasonication, has also been found to achieve selective lithium recovery with improved efficiency and selectivity [10,11]. Emerging techniques such as contact-electro-catalysis, deep eutectic solvent leaching, and photocatalysis have further improved Li and Co recovery while reducing chemical consumption and environmental impact [12–14]. Antisolvent precipitation, hydrometallurgical–pyrometallurgical strategies, and ultrasound-assisted black mass leaching have been applied for selective extraction of multiple metals from NMC-type cathodes [15,16]. Similar approaches have also been extended to mixed anode–cathode materials, achieving efficient recovery of Li, Co, Ni, and Mn [17]. In addition, microemulsion-based extraction enables high-purity cobalt recovery with excellent recyclability [18]. Although these studies demonstrate high recovery efficiencies through experimental process development, predictive understanding of how process parameters influence metal recovery remains limited, particularly when attempting to integrate mechanistic insights with flexible modeling approaches.

In recent years, machine learning techniques have gained increasing attention as analytical tools for modeling complex nonlinear relationships in chemical and metallurgical processes [19–21]. Data-driven models can capture interactions among multiple process parameters and provide predictive insights that support process optimization [22, 23]. Recent studies have also demonstrated the application of physics-informed neural networks (PINNs) to chemical and metallurgical process modeling. A PINN based Population Balance Equations model was developed for analyzing Gibbsite crystallization dynamics by incorporating population balance equations into NN training to provide a more robust alternative to purely data-driven predictive models for process control [24]. PINNs have also been applied to chemical reaction kinetics, where a causal PINN was used in solving mass-action-based ordinary differential equations and estimate unknown reaction-rate parameters while maintaining physically consistent concentration trajectories [25]. Wang et. al. developed an AI-based controller by incorporating a PINN environment for crude distillation [26]. It was shown that the model was able to reduce monotonicity violations while maintaining prediction accuracy. Beyond process operations, a PINN framework for molecular solubility prediction incorporated with thermodynamic constraints into neural-network training [27], was deployed for improving the extrapolation performance compared with conventional neural networks. Similarly, a PINN combined with sparse identification of nonlinear dynamical systems was used to model adsorption kinetics in metal-oxide gas sensors, enabling extraction of interpretable adsorption/desorption parameters and reconstruction of hidden adsorption dynamics [28]. These studies demonstrate that incorporating domain-specific information into neural networks can improve their predictive capability and physical consistency. Beyond these PINN-based approaches, conventional response surface models (RSM) use predefined polynomial relationships and may have limited flexibility in capturing complex nonlinear interactions among process variables. Machine learning models can complement this limitation by learning nonlinear relationships directly from experimental data without imposing a fixed polynomial structure.

In this study, four supervised machine learning models – linear regression (LR), a second order quadratic polynomial regression (QPR), neural network (NN), and random forest (RF) – were developed to model the relationship between leaching process parameters and the recovery efficiencies of Li and Co using the experimental data reported in Ref. [29]. In addition, the response surface model (RSM) reported in ref. [29] was also incorporated into the proposed RSM-enhanced neural network (RSM-NN) framework as an empirical prior during NN training. The RSM-NN combines data-driven learning from the experimental observations with the empirical relationships captured by the previously established RSM model. All models were implemented in Python using the Scikit-learn library [30]. By combining empirical guidance with data-driven learning, the proposed approach aims to improve predictive

accuracy relative to conventional empirical and standalone data-driven models while maintaining consistency with the trends captured by the RSM model.

1.1. Dataset Description and Preprocessing

The dataset used in this study was adopted from a previous experimental investigation on ultrasound-assisted leaching of Li and Co from spent LIBs [29]. In the original study, experimental investigations were conducted and the resulting data were used to develop an RSM model for predicting metal recovery efficiencies. The experiment used spent LCO cathode material, with the elemental composition of the cathode powder reported as 3.40 wt% Li, 12.38 wt% Co, 0.01 wt% Mn, 0.02 wt% Ni and 0.05 wt% Cu [29]. The black powder underwent pretreatment involving discharge, manual disassembly, binder removal, washing, filtration, and drying prior to leaching. Gluconic acid was used as the leaching agent, with a concentration range of 0.1–0.5 mol/L and a liquid-to-solid ratio of approximately 66.7 mL/g. Ultrasonic irradiation was performed using a Hybrid MW-US high-pressure chemical reactor at a frequency of 20 kHz, with the equipment power setting varied from 10% to 50%, corresponding to the 100–500 W power values as reported in ref. [29]. The three process parameters varied in the experimental study, namely ultrasound power (%), reaction temperature (°C), and leaching time (min), were used as input variables for the machine-learning models, while Li (Y_{Li}) and Co (Y_{Co}) recovery efficiencies were used as response variables. The temperature ranged from 120 °C to 220 °C and the reaction time varied between 20 min and 120 min. The ultrasound power ranged from 10% to 50% in the original study, which did not report a separate ultrasonic power calibration procedure. Therefore, the ultrasound-power variable in the present study represents the equipment settings and corresponding power values reported for the experimental system in ref. [29]. Additionally, since the present study directly uses the experimental dataset reported in [29], variables such as leaching-agent concentration, liquid-to-solid ratio, particle size, and acidity were not independently varied and were therefore not included as predictive variables. The dataset consisted of 180 experimental observations. The descriptive statistics of the input and response variables are presented in Table 1. Prior to model development, the dataset was pre-processed to ensure consistency and to confirm that all variables were represented in numerical format suitable for machine learning analysis. The dataset was then divided into training and testing subsets by randomly assigning 80% of the dataset for training and the remaining 20% for testing. The testing dataset was kept separate during machine-learning model training to evaluate the predictive performance of the developed models.

At first, four supervised machine learning algorithms were considered, viz. LR, QPR, NN, and RF. Following this, an RSM-NN model was formulated using the previously established RSM model from [29] as an empirical baseline within a residual neural-network framework. In the RSM-NN model, the NN learns a residual correction to the RSM prediction, while an additional RSM-based regularization term encourages the final predictions to remain close to the empirical RSM relationship. Thus, the proposed framework combines direct data-driven learning from the experimental observations with empirical information

Table 1
Descriptive statistics of dataset used in the present study.

Metrics	Power (%)	Temperature (°C)	Time (min)	Y_{Li} (%)	Y_{Co} (%)
count	180.00	180.00	180.00	180.00	180.00
mean	30.00	170.00	70.00	79.54	75.23
std	14.18	34.25	34.25	17.03	16.49
min	10.00	120.00	20.00	37.14	34.73
25%	20.00	140.00	40.00	68.58	64.10
50%	30.00	170.00	70.00	84.39	79.74
75%	40.00	200.00	100.00	94.23	89.10
max	50.00	220.00	120.00	99.20	98.17

provided by the previously established RSM model [29]. To improve model robustness, five-fold cross-validation (CV) was applied during the training phase. This procedure evaluates the models across multiple training-validation partitions of the dataset, thereby reducing dependence on a single data split. The performance of the models was ultimately assessed using the held-out test dataset. Feature scaling was applied to the NN and RSM-NN models to facilitate stable NN training. In contrast, scaling was not applied to the LR and RF models. The predictive performance of the developed models was evaluated using the coefficient of determination (R^2) and the root mean square error (RMSE). The developed models are intended for the experimental conditions represented in the dataset and might not be directly transferable to other ultrasonic equipment or operating systems without further experimental validation.

1.2. Performance Analysis of Supervised Learning Models

This section presents a comparative analysis of four supervised machine learning models, namely LR, QPR, NN, and RF, applied to the LIB leaching dataset. The models exhibited different predictive capabilities depending on their ability to represent the relationships between the process variables and metal recovery efficiencies. The LR model assumes a purely linear relationship between the input variables and response outputs and showed the lowest predictive performance among the evaluated models. The LR model achieved R^2 values of 0.797 ± 0.065 for Li and 0.877 ± 0.037 for Co, indicating that a purely linear formulation is insufficient to adequately represent the relationships present in the dataset.

To account for nonlinear relationships while retaining a polynomial formulation, a second-degree QPR model was also evaluated. Unlike LR, the QPR model incorporates squared terms and pairwise interaction terms between the process variables, allowing it to represent curvature and nonlinear interactions in the response surface. The QPR model achieved R^2 values of 0.941 ± 0.017 for Li and 0.966 ± 0.010 for Co, representing a clear improvement over the LR model. The improvement indicates that incorporating second-order terms provides a better representation of the response relationships than the purely linear formulation.

The NN consisted of two hidden layers with 16 and 8 neurons,

respectively, using the rectified linear unit (ReLU) activation function. The model was trained using the Adam optimizer with an adaptive learning rate of 0.01, and a maximum of 5000 training iterations. The NN achieved R^2 values of 0.940 ± 0.030 for Li and 0.959 ± 0.019 for Co. These results are comparable to those obtained using QPR, indicating that both approaches were able to represent nonlinear relationships in the experimental dataset. The RF model was implemented using an ensemble of 10 decision trees and achieved R^2 values of 0.986 ± 0.006 for Li and 0.988 ± 0.006 for Co, giving the highest predictive performance among the standalone data-driven models. The hyperparameter configurations used for the NN and RF models were selected based on prior optimization experiments (illustrated in the Appendix) and were kept fixed during the comparative evaluation. The strong performance of the RF model may be attributed to its ability to capture nonlinear relationships and interactions within the experimental dataset without imposing a predefined functional form.

The plots of the predicted versus actual values for LR, QPR, NN, and RF are shown in Figs. 1–4, respectively. These plots provide visual confirmation of the quantitative performance metrics. The LR model exhibits greater scatter around the diagonal line (Fig. 1), reflecting its limited ability to represent nonlinear relationships between the input variables and the leaching efficiencies. These deviations from the ideal agreement line represent prediction errors, with the greater dispersion indicating lower agreement between the predicted and actual values and, consequently, lower prediction accuracy compared with the other models. The QPR model produces predictions that are more closely distributed around the diagonal line (Fig. 2), consistent with its improved R^2 values due to the inclusion of second-order and interaction terms. The NN provides a similar level of agreement with the experimental values (Fig. 3), although some deviations from the ideal agreement line remain. These deviations represent residual prediction errors and indicate that the NN does not reproduce every experimental observation exactly. However, the relatively limited scatter around the diagonal line, together with its R^2 and RMSE values, indicates good predictive accuracy and consistent performance across the evaluated data. The RF model exhibits the closest agreement with the ideal one-to-one relationship, with relatively minor dispersion around the diagonal line (Fig. 4). The small deviations from the ideal line represent residual prediction errors, while the limited dispersion indicates high agreement

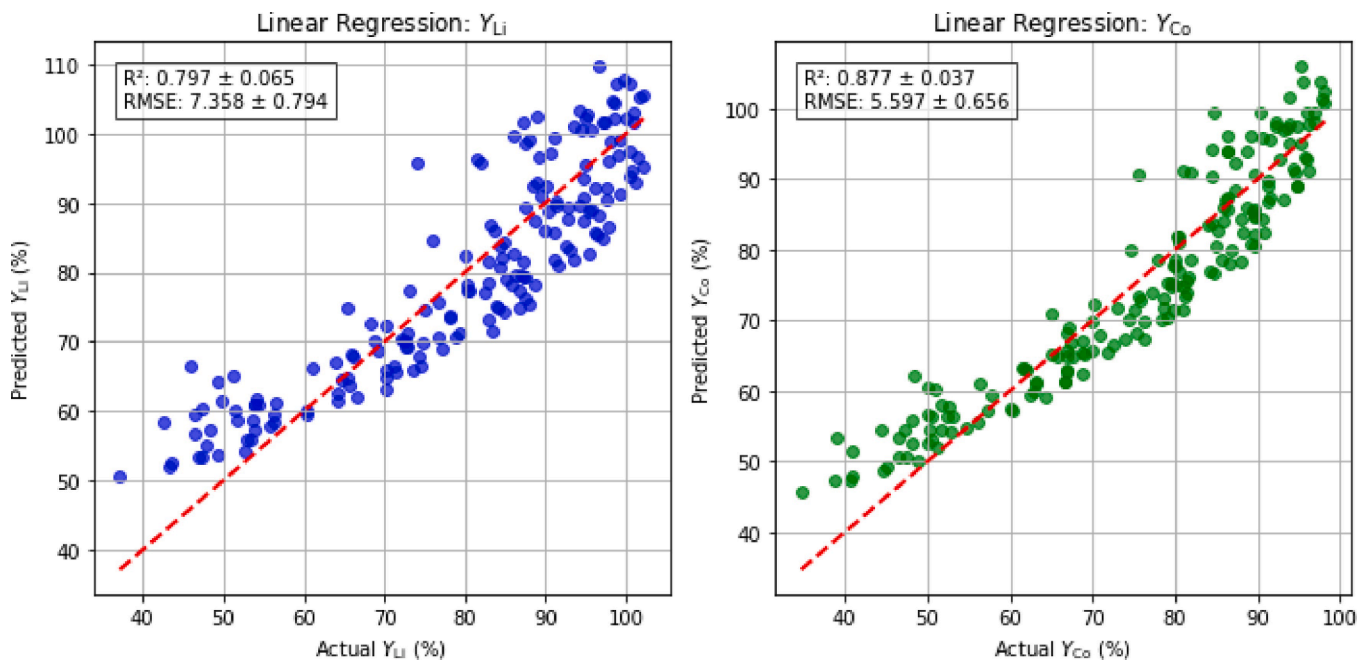


Fig. 1. Plot of predicted vs. actual for the LR model.

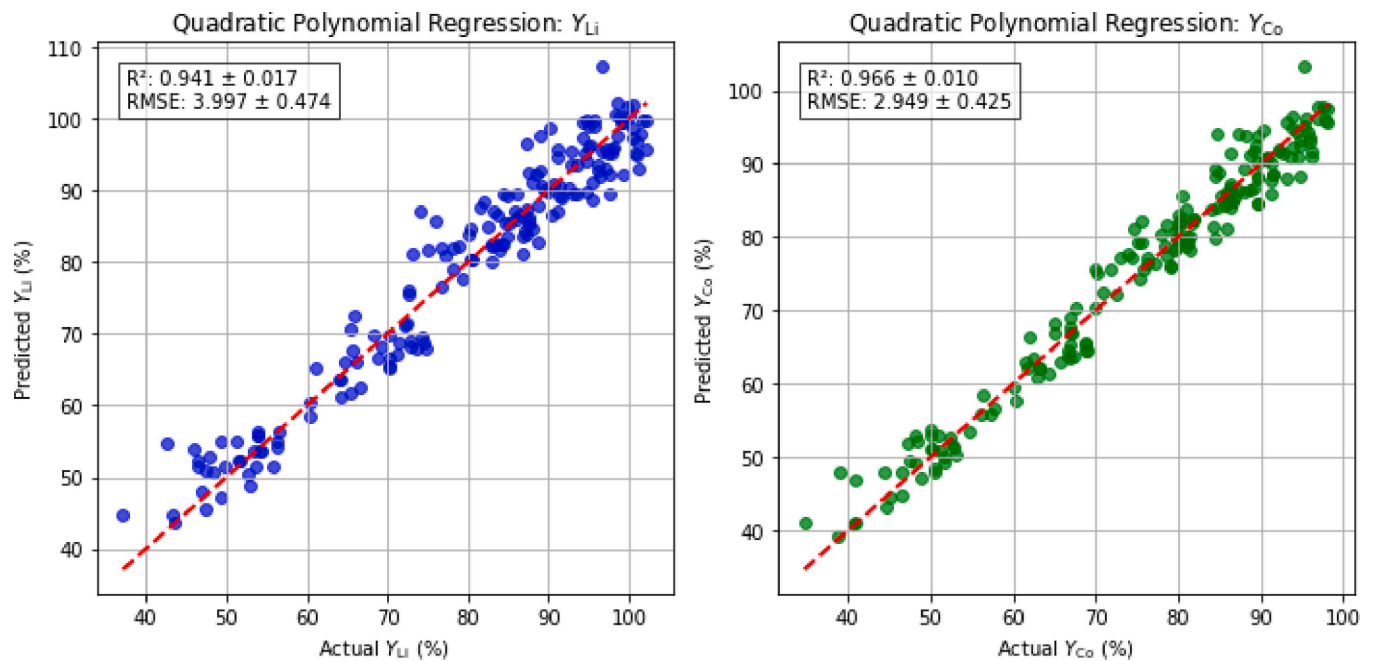


Fig. 2. Plot of predicted vs. actual for the QPR model.

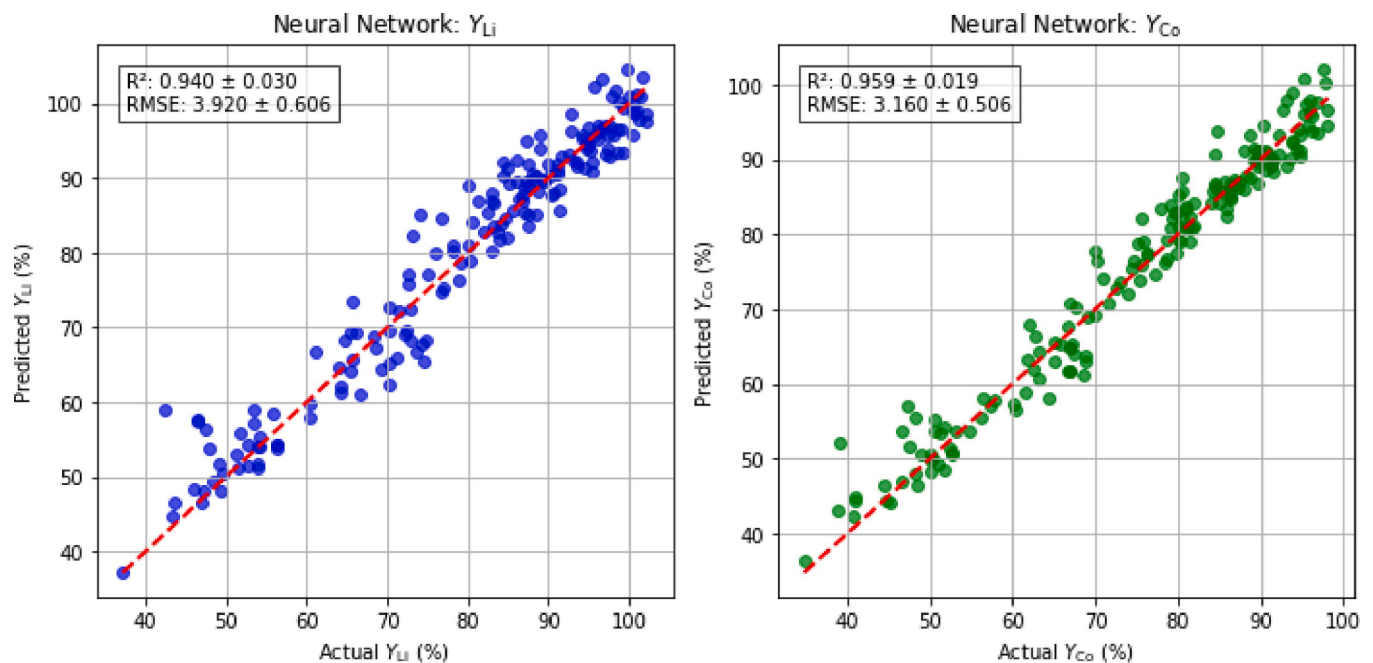


Fig. 3. Plot of predicted vs. actual for the NN model.

between the predicted and actual values and therefore strong predictive accuracy. Together with the high R^2 and low RMSE values obtained across the CV folds, the limited scatter also indicates consistent model performance. Overall, the results show that increasing model flexibility from a linear formulation to quadratic, neural-network, and ensemble-based approaches improves the ability to represent the relationships observed in the experimental dataset, with RF providing the strongest predictive performance among the standalone models.

1.3. Response Surface Model-integrated Neural Network Approach

The RF model achieved the highest predictive accuracy among the

purely data-driven approaches. However, it does not explicitly incorporate the empirical process relationships identified from the leaching experiment. To address this limitation, the quadratic RSM from the original experimental study [29] was incorporated as an empirical prior within the NN model. The overall conceptual framework, including 5-fold training and RSM-based regularization, is illustrated in Fig. 5. The RSM model in ref. [29] was fitted to the same 180 experimental observations used in the present work. In this study, the experimental dataset itself was used as input for training the machine learning models, while the previously reported RSM equation was incorporated into the RSM-NN framework to provide empirical guidance. The RSM-NN architecture consisted of five layers with 3, 64, 64, 32, and 2 neurons,

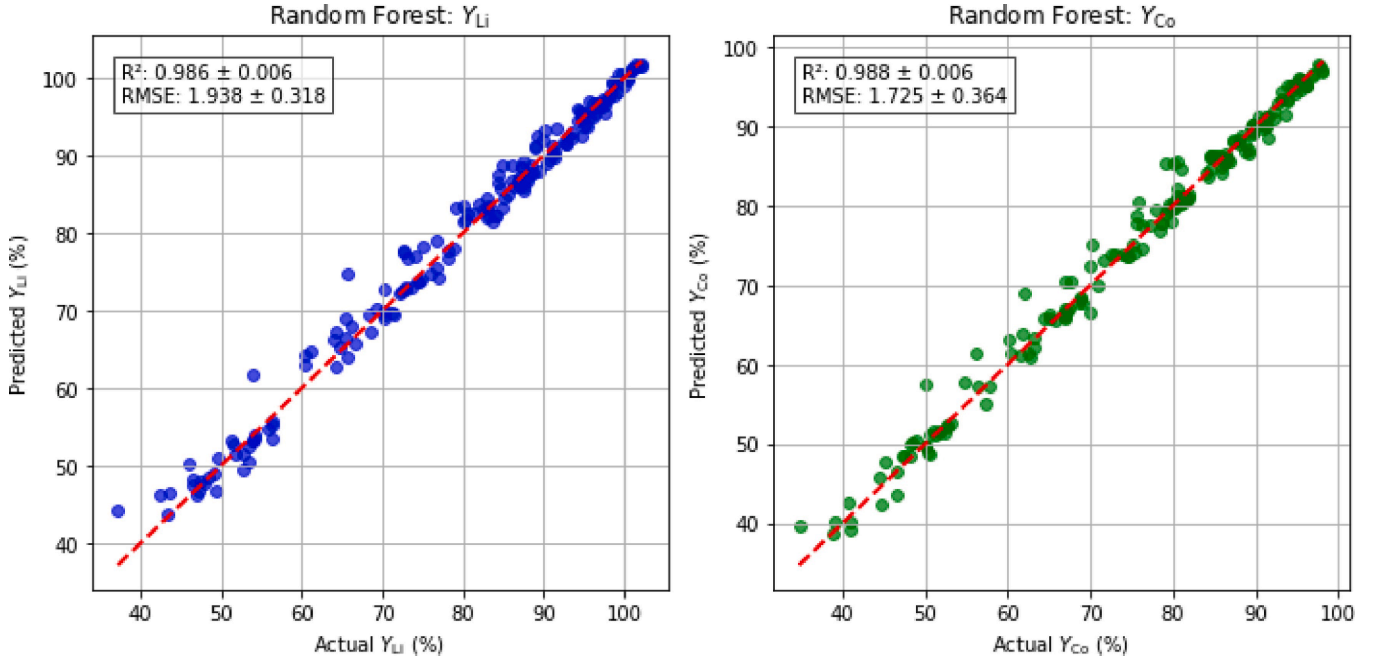


Fig. 4. Plot of predicted vs actual for the RF model.

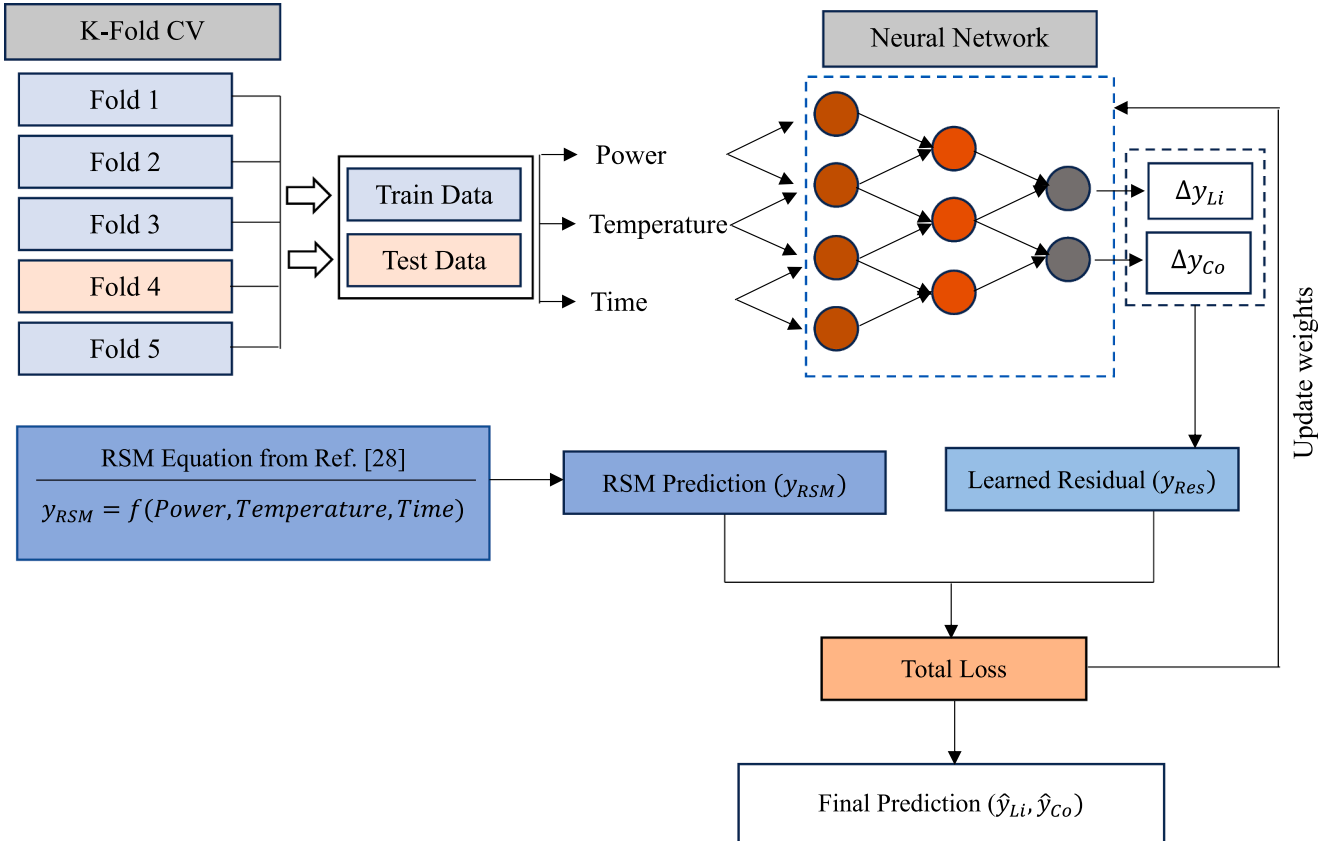


Fig. 5. RSM-NN framework implemented in the present study.

using ReLU activation in the hidden layers. Training was performed using a composite loss function that simultaneously minimized the prediction error relative to the experimental observations and the deviation from the RSM constraint. Instead of predicting the leaching efficiencies directly, the network was trained to learn a residual function

relative to the RSM predictions, allowing it to refine prior trends while capturing additional nonlinearities in the data. The relatively small experimental dataset was addressed through five-fold CV, which was used to evaluate model performance across multiple training and validation subsets rather than relying on a single data partition. The

RSM-based regularization also constrains the residual learning process by penalizing deviations from the established empirical RSM relationship.

The RSM equations reported in Ref. [28] were incorporated into the proposed RSM-NN framework as the empirical baseline for predicting Li and Co leaching efficiencies, as illustrated in Fig. 4. The RSM formulations for Li (y_{LiRSM}) and Co (y_{CoRSM}) are respectively defined by Eqs. (1) and (2) as [29]:

$$y_{LiRSM} = 92.70 + 4.23A + 3.63B + 21.84C - 1.47AB + 0.9962AC + 2.43BC - 5.43A^2 - 7.90B^2 - 14.49C^2 \quad (1)$$

$$y_{CoRSM} = 85.09 + 3.71A + 4.60B + 21.91C - 0.7750AB + 2.31AC - 0.8275BC - 3.97A^2 - 5.5B^2 - 11.30C^2 \quad (2)$$

where A , B , and C represent ultrasound power, reaction temperature, and leaching time, respectively.

In the proposed RSM-NN framework, the NN does not directly predict the final Li and Co recovery efficiencies. Instead, it learns a residual correction to the RSM predictions. For each response, the final prediction is therefore formulated as,

$$y_{Final\ prediction} = y_{RSM} + y_{Residual_{NN}}$$

where $y_{Residual_{NN}}$ represents the residual learned by the NN. This residual formulation allows the NN to learn deviations from the empirical relationships established by the RSM while retaining the trends captured by the previously developed model.

Fig. 6 depicts the plot of predicted leaching efficiencies against actual observations along with a reference line representing an exact match between predicted and experimental values. It can be seen that the RSM-NN framework demonstrated excellent agreement with the experimental observations, achieving R^2 values of approximately 0.999 for both Li and Co with negligible standard deviations, indicating strong stability (Fig. 6). The small deviations of the predicted values from the 45° reference line represent the residual prediction errors of the model and indicate that the predictions closely follow the experimental observations across the investigated range. The limited scatter around the reference line, together with the high R^2 values and low RMSE values, indicates high predictive accuracy and consistent performance, although these results should be interpreted within the range of experimental conditions represented in the dataset. These results highlight the advantage of integrating established empirical relationships with data-driven learning: the RSM-NN leverages the trends captured by the RSM while improving predictive accuracy through residual learning. The resulting model produces smooth and consistent response patterns and demonstrates the capability to capture both the dominant trends represented by the RSM and additional nonlinear variations in the leaching behavior of Li and Co from spent LIBs.

1.4. Model Performance and Partial Dependency Analysis

Following the development of the RSM-NN framework, the predictive performance of all models was systematically compared to evaluate their capability in representing the leaching behavior of Li and Co. The leaching process was modeled using four supervised learning approaches: LR, QPR, NN, RF, and the integrated RSM-NN. Table 2

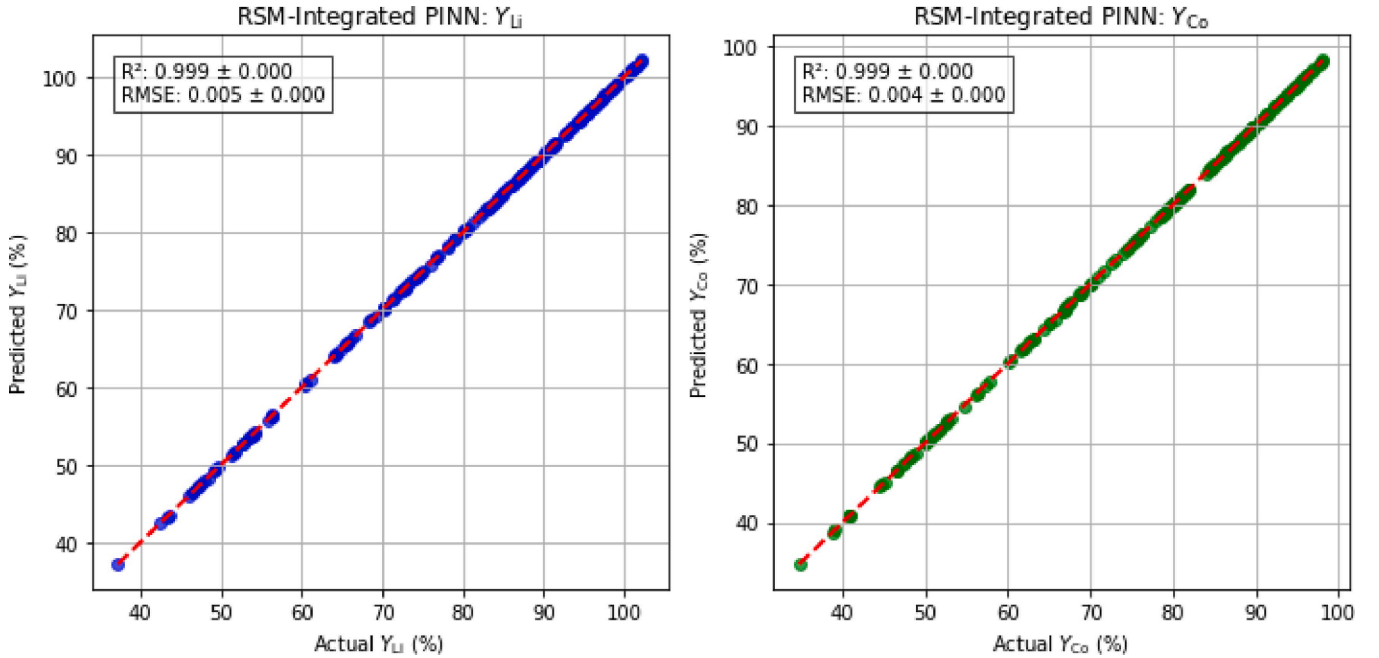


Fig. 6. Plot of predicted vs actual for the RSM-integrated PINN model.

Table 2

Performance comparison of the predictive models for Li and Co recovery (The values represent mean $\pm$ standard deviation obtained from 5-fold CV).

Metrics	R^2 (Li)	R^2 (Co)	RMSE (Li)	RMSE (Co)
RSM [29]	0.989	0.965	2.110	3.600
LR	0.797 ± 0.065	0.877 ± 0.037	7.358 ± 0.794	5.597 ± 0.656
QPR	0.941 ± 0.017	0.966 ± 0.010	3.997 ± 0.474	2.949 ± 0.425
NN	0.940 ± 0.030	0.959 ± 0.019	3.920 ± 0.606	3.160 ± 0.506
RF	0.986 ± 0.006	0.988 ± 0.006	1.938 ± 0.318	1.725 ± 0.364
RSM-NN	0.999 ± 0.000	0.999 ± 0.000	0.005 ± 0.000	0.004 ± 0.000

summarizes the performance metrics of these models alongside the metrics of the RSM from the original study [29]. The RSM-NN framework provides an additional modeling capability beyond the standalone NN by using the established RSM relationship as an empirical baseline and learning a residual correction from the experimental data. While the standalone NN directly learns the relationship between the process variables and metal recovery, the RSM-NN decomposes the prediction into the RSM contribution and a learned residual component. Therefore, deviations between the predicted and actual values arise from the residual prediction error that remains after the RSM contribution and the learned correction are combined. These deviations are expected because the model does not reproduce every experimental observation exactly and reflect the remaining prediction error of the model. The relatively small deviations, together with the R^2 and RMSE values, indicate high predictive accuracy and reliable agreement with the experimental data. The RSM-NN achieves an R^2 of 0.999 for both Li and Co recovery efficiencies, compared with R^2 values of 0.989 and 0.962 for Li and Co, respectively. This corresponds to an increase of 0.010 in R^2 for Li and 0.037 for Co from the RSM model reported in the original study [29]. The resulting improvement in predictive performance demonstrates the potential benefit of integrating an established empirical model with residual NN learning.

The RSM constraint also serves as a regularization mechanism, encouraging predictions to remain consistent with the empirical process trends captured by the RSM model across the design space. The RSM-NN model therefore combines the flexibility of data-driven learning with empirical information captured by the established RSM, resulting in high predictive accuracy and stability across the evaluated models. The superior performance of the RSM-NN model is further illustrated through partial dependency plots (PDPs) of Li and Co recovery efficiencies. The dependency of recovery efficiency on power and temperature at a fixed time of 70 min (Fig. 7) reveals a well-defined optimal region, with both Li and Co recoveries increasing with temperature and ultrasonic power before approaching a plateau. The combined response indicates an interaction between power and temperature, with the recovery efficiency depending on their combined operating levels and showing diminishing returns as both parameters increase. The time-temperature PDP at a fixed power of 30% (Fig. 8) shows that recovery efficiencies rise rapidly with time and achieve near-complete extraction

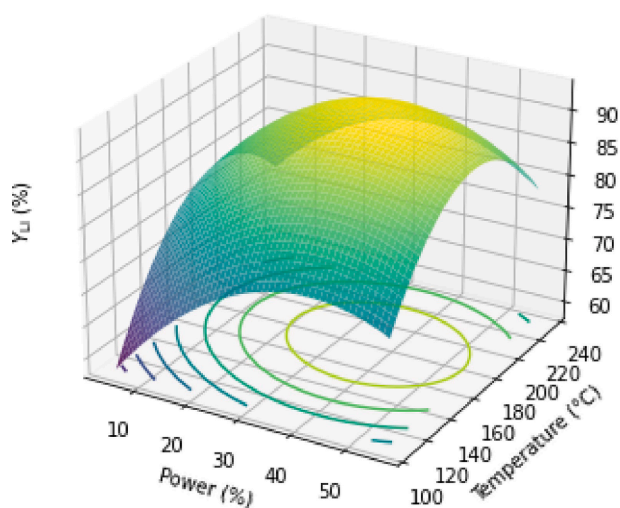
within a relatively short duration, while the influence of temperature is more gradual. This indicates that at the fixed power level of 30%, reaction time has a stronger influence on recovery than temperature within the explored operating range, while the combined variation of time and temperature contributes to the observed recovery response. Similarly, the power-time PDP (Fig. 9) demonstrates that recovery efficiencies increase primarily with time, whereas ultrasonic power exerts a weaker influence.

The smooth and consistent trends observed in these PDPs provide an interpretable representation of the modeled relationships without the spurious fluctuations often seen in purely data-driven models. These trends are qualitatively consistent with the experimental observations and the empirical relationships represented by the RSM; however, the PDPs alone do not constitute independent validation of the underlying chemical or kinetic mechanisms. Overall, the results demonstrate a clear progression in modeling capability: from the underfitting LR model to the more flexible OPR, NN and RF models, and finally to the RSM-NN. The RSM-NN integrates data-driven learning with RSM-based constraints to achieve both high predictive accuracy and improved interpretability of the leaching process. Although it demonstrates very high accuracy and stability across 5-fold CV, its performance primarily reflects the strength of the hybrid modeling framework, with the RSM providing empirical guidance from the same dataset.

2. Conclusion

This study focused on analyzing the predictive performance of selected machine learning models on the ultrasound-assisted leaching efficiencies of Li and Co from spent LIBs. Four standalone supervised learning approaches, LR, QPR, NN, and RF, were firstly evaluated using the experimental data sourced from a prior research study. Furthermore, an RSM-NN modeling framework was formulated by incorporating the RSM formulation as an empirical constraint during training. The resulting model captured the nonlinear relationships between ultrasonic power, temperature, and leaching time, providing a flexible data-driven representation while maintaining consistency with the empirical trends captured by the RSM model. Overall, the results highlight the potential of RSM-informed machine learning frameworks to complement conventional RSM models by improving predictive modeling of complex

PDP: Y_{Li} vs Power-Temperature (Time = 70 min)



PDP: Y_{Co} vs Power-Temperature (Time = 70 min)

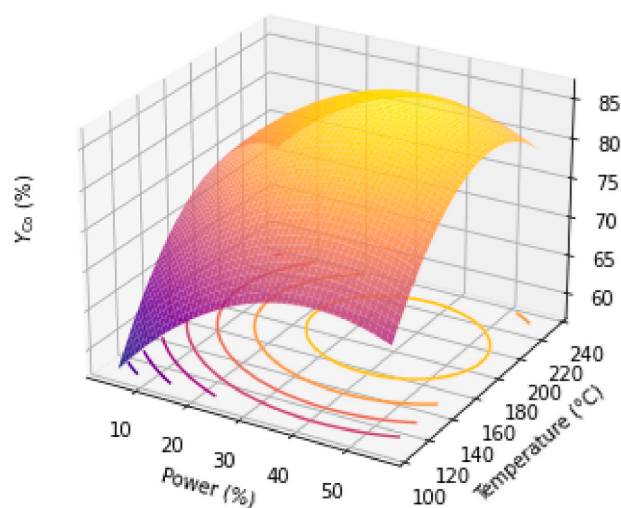


Fig. 7. PDP of metal recovery efficiencies with power and temperature at fixed time of 70 min.

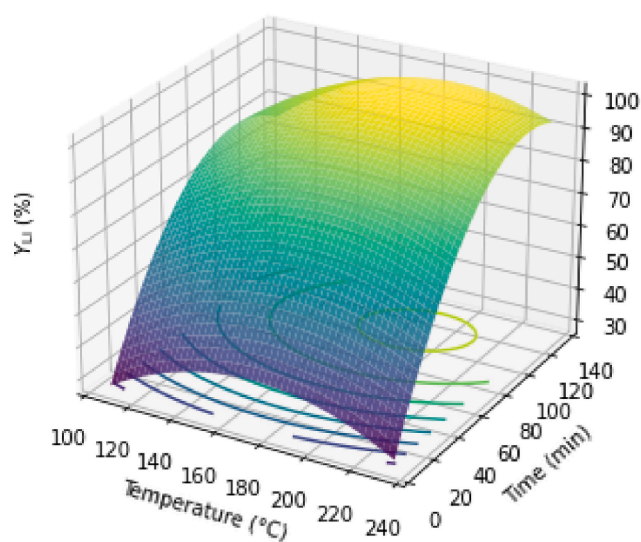
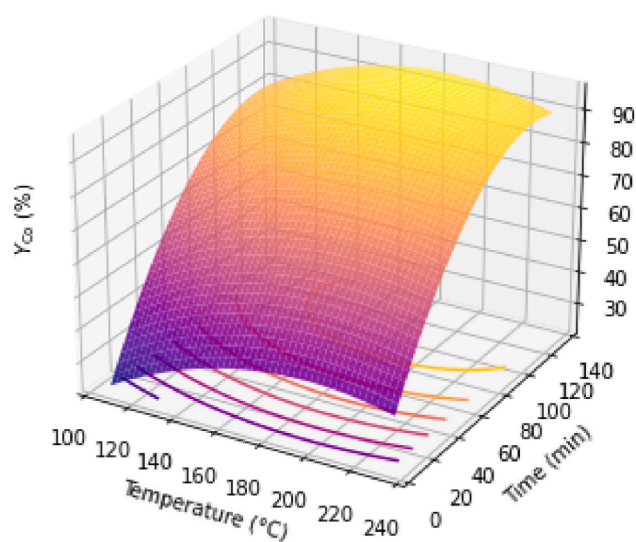
PDP: Y_{Li} vs Time-Temperature (Power = 30%)PDP: Y_{Co} vs Time-Temperature (Power = 30%)

Fig. 8. PDP of metal recovery efficiencies with time and temperature at fixed power of 30%.

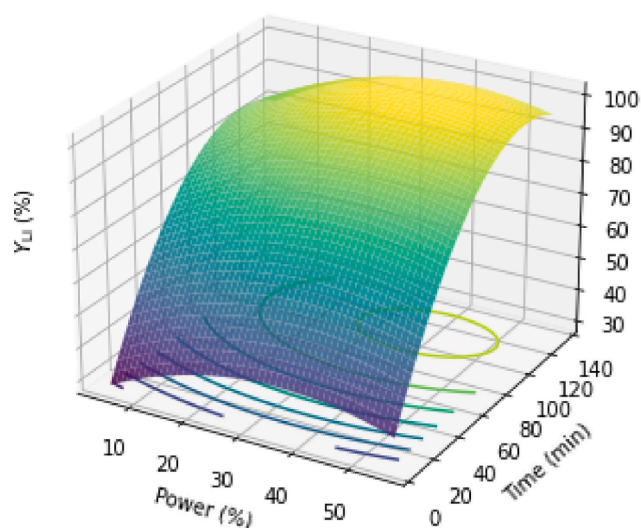
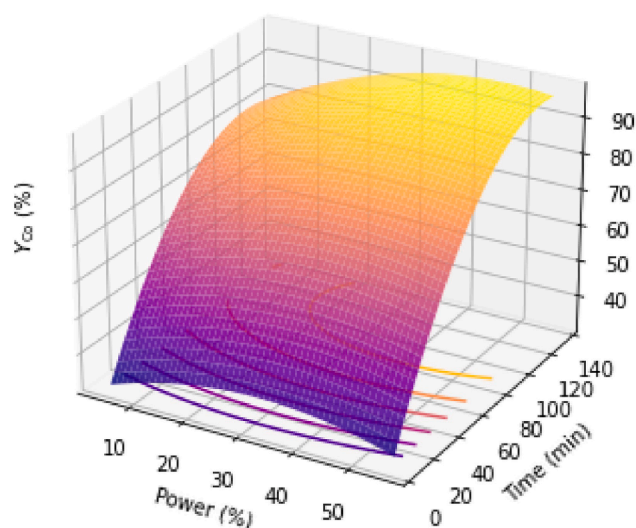
PDP: Y_{Li} vs Power-Time (Temp=170°C)PDP: Y_{Co} vs Power-Time (Temp=170°C)

Fig. 9. PDP of metal recovery efficiencies with power and time at fixed temperature of 170 °C.

nonlinear relationships and providing valuable insights for optimizing metal recovery processes from spent LIBs. It is anticipated that the present RSM-NN framework can support improved understanding and optimization of metal recovery processes from spent LIBs by providing reliable predictive tools for analyzing the influence of key operating parameters. Future work will investigate the effects of acidification and NaOH concentration on the resulting precipitation behavior and metal recovery.

CRediT authorship contribution statement

Y. Bhalerao: Supervision, Data curation. **Liang Gao:** Supervision,

Project administration. **A. Garg:** Visualization, Investigation, Conceptualization. **V. Vijayaraghavan:** Writing – original draft, Software, Methodology.

Funding declaration

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Declaration of Competing Interest

There are no relevant financial or non-financial competing interests to report.

Appendix

Hyperparameter Selection for NN model:

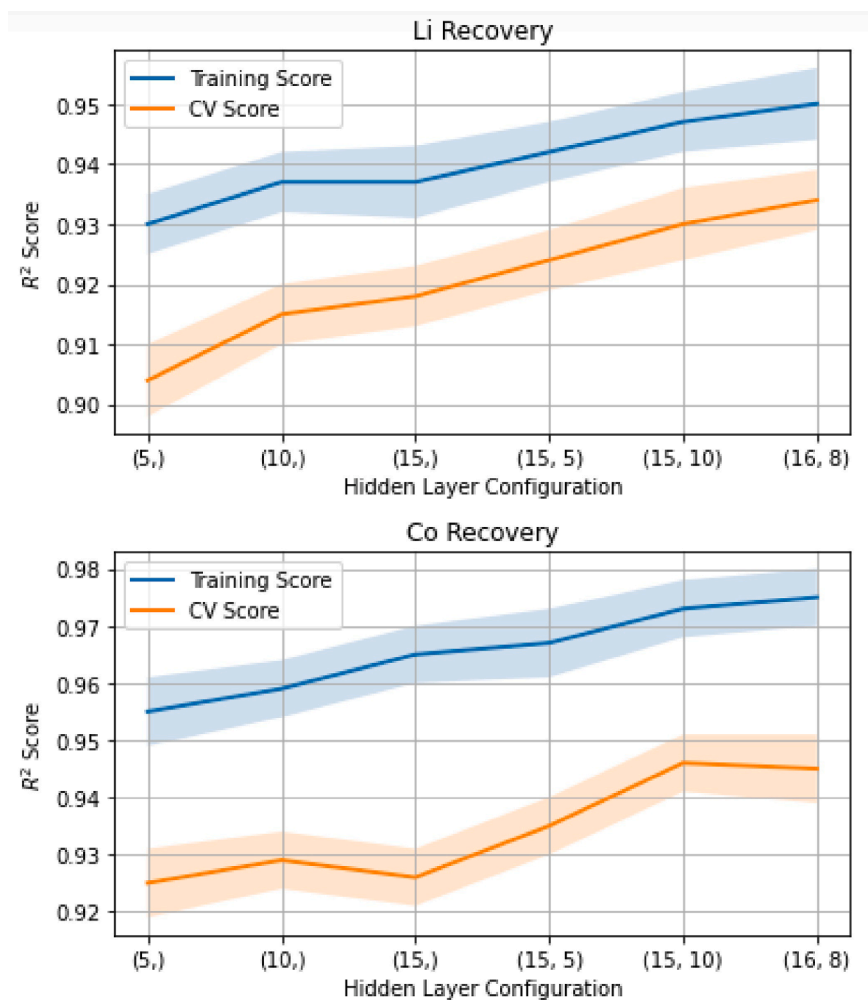


Figure A1. Effect of hidden-layer configuration on training and CV R^2 scores for Li and Co recovery

The results from Fig. A1 shows that the (16, 8) hidden-layer configuration provides the highest CV R^2 for Li and a comparable high CV performance for Co. Therefore, the (16, 8) configuration was selected for the NN model.

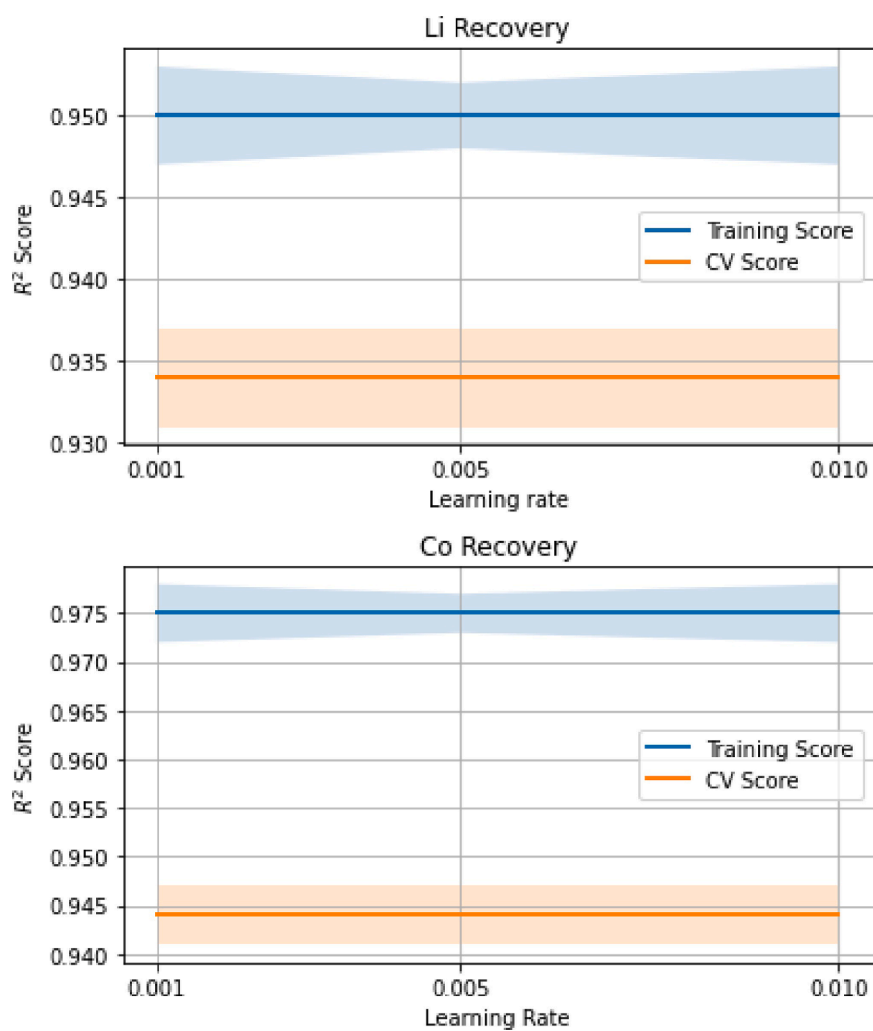


Figure A2. Effect of learning rate on training and CV R^2 scores for Li and Co recovery

The training and CV R^2 scores remained essentially unchanged across the evaluated learning rates as depicted in Fig. A2. A learning rate of 0.1 was selected for the final NN configuration because it provided faster training while maintaining comparable predictive performance.

Hyperparameter selection of RF model:

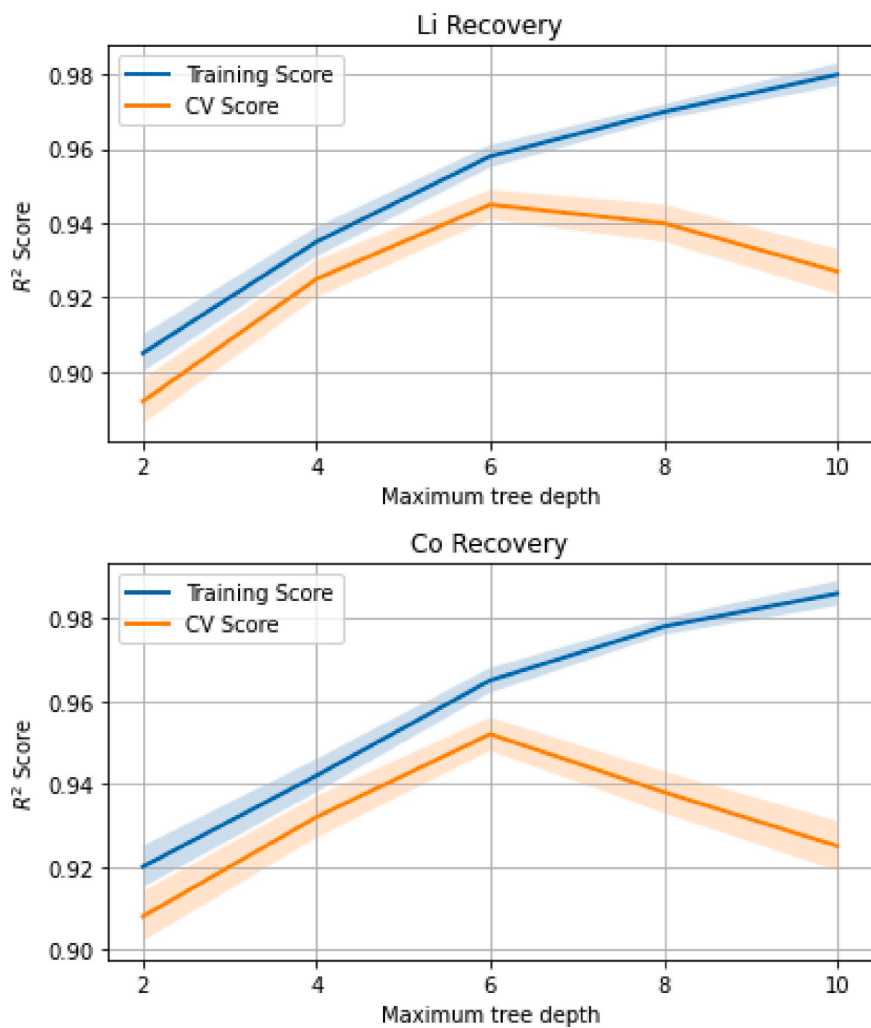


Figure A3. Effect of Maximum Tree Depth on Training and CV R^2 Scores for Li and Co Recovery

Fig. A3 shows that the CV R^2 scores increase as the maximum tree depth increases initially, reaching the highest performance at a maximum tree depth of 6 for both Li and Co recovery. Further increasing the tree depth results in a decrease in CV performance, despite continued improvement in the training R^2 . Therefore, a maximum tree depth of 6 is selected for the RF model as it provided the highest CV performance for both responses while avoiding the decline observed at greater depths.

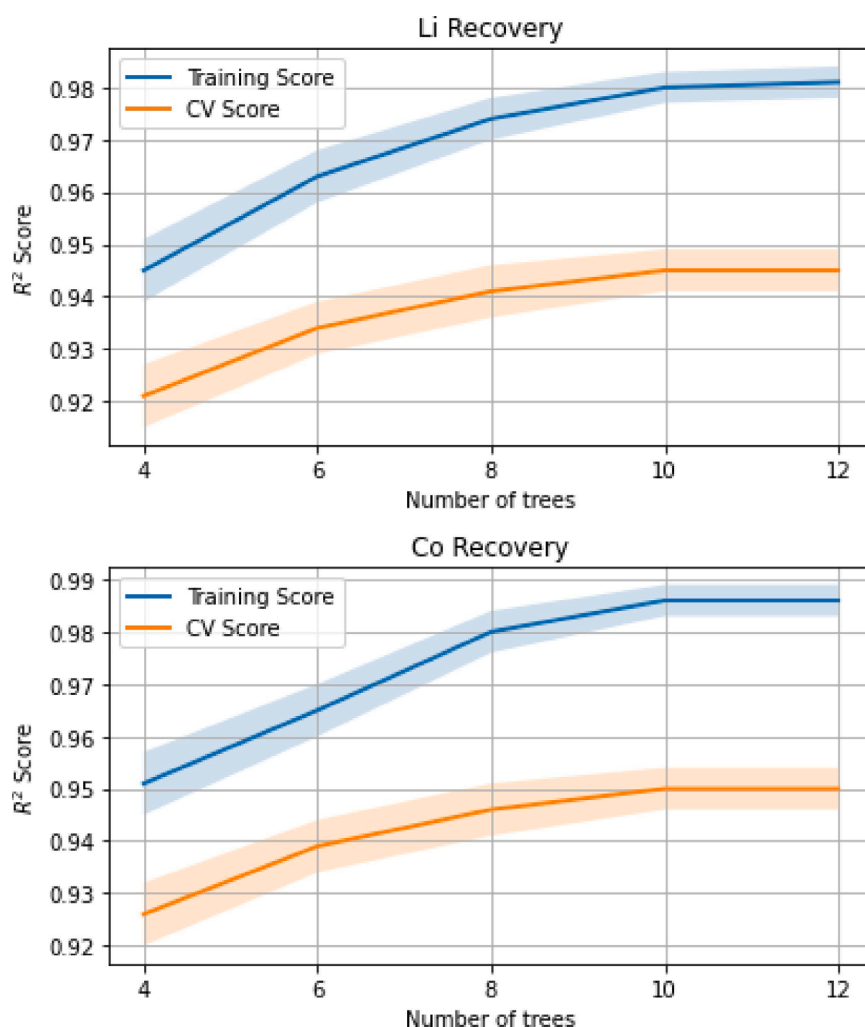


Figure A4. Effect of Number of Trees on Training and CV R^2 Scores for Li and Co Recovery

The CV R^2 scores increase as the number of trees increases, with the highest performance reached at approximately 10 trees for both Li and Co recovery (Fig. A4). Increasing the number of trees beyond 10 provides no further improvement in CV performance, while the training R^2 continues to increase slightly. Therefore, 10 trees were selected for the final RF model as it provides the highest CV performance without unnecessary increases in model complexity.

Data availability

Data will be made available on request.

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