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Interpretable modeling of metallurgical responses for an industrial coal column flotation circuit by XGBoost and SHAP-A "conscious-lab" development

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ABSTRACT

Surprisingly, no investigation has been explored relationships between operating variables and metallurgical responses of coal column flotation (CF) circuits based on industrial databases for under operation plants. As a novel approach, this study implemented a conscious-lab "*CL*" for filling this gap. In this approach, for developing the *CL* dedicated to an industrial CF circuit, SHapley Additive exPlanations (SHAP) and extreme gradient boosting (XGBoost) were powerful unique machine learning systems for the first time considered. These explainable artificial intelligence models could effectively convert the dataset to a basis that improves human capabilities for better understanding, reasoning, and planning the unit. SHAP could provide precise multivariable correlation assessments between the CF dataset by using the Tabas Parvadeh coal plant (Kerman, Iran), and showed the importance of solid percentage and washing water on the metallurgical responses of the coal CF circuit. XGBoost could predict metallurgical responses (R-square > 0.88) based on operating variables that showed quite higher accuracy than typical modeling methods (Random Forest and support vector regression).

1. Introduction

Column flotations (CFs) are completely different units in designing and operating compare to the conventional mechanical flotation cells. CFs could efficiently upgrade fine particles' concentration at one cleaning step, while mechanical cells would require sequential steps [1–3]. In general, CFs have some advantages over conventional cells, such as lower capital and operating cost, less wear (no moving parts), lower floor space, easier control, and simpler circuits. Since there is no mechanical agitation in the CFs there are limited variables for controlling the systems (flow rates, feed air, wash water, bubble size, reagent dosages, and air holdup) [1–6]. Therefore, modeling such a process could significantly improve its performance.

Bouchard et al. [7] provided a dynamic theoretical simulation of CF. This framework focused on water, solids, and gas flows and their impact on the pulp level and output flow rates. They took many variables constant and emphasized that although their outcomes were qualitatively reliable, only a comprehensive empirical assessment would determine the accuracy of their approach and identify required improvements [7]. An overview for assessing the CF simulation and control has been indicated that their potential is not exploited even after many years of installation in mineral processing units. It was highlighted that considering the multivariate statistical assessments could be a key for monitoring CF units [8]. Maldonado et al. [9] used froth depth, collection zone gas holdup, and bias rate for developing a predictive model to control a CF at COREM (Mineral Processing Research Consortium) pilot plant in Québec City, Canada. It was reported that bubble size distribution (BSD) could be used to control recovery for a given particle size distribution in a two-phase pilot CF [10]. Núñez et al. [11] used a hierarchical hybrid fuzzy strategy to control ten cleaning FCs. However, just a few investigations have been considered modeling that related to the CF operations based on the industrial datasets (published explorations mainly focused on the small scales) [12–14].

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As a new approach, conscious-lab "*CL*" could be a tactical plan for tackling this gap. *CL* uses existing monitored data collected from industrial plants for generating explainable AI (EAI) models. This strategic approach can develop an accurate dynamic AI system that reduces laboratory work costs, removes the scale-up challenges, saves time, and makes decisions based on the plant's actual operational properties (not based on the ideal theoretical aspect) [15–21]. Nakhaeie et al. [22,23] employed a multi-layer feed-forward neural network (FANN) to predict a CF's metallurgical performance using Sarcheshmeh copper samples. They concluded that using artificial intelligence (AI) systems based on industrial datasets could help the process optimization without conducting laboratory experiments. However, since FANN could not provide any insight about relationships between process variables and their representative responses should be classified as a black box AI system (not as an EAI system). A robust EAI system should illustrate the relationship between each record of variables with their representative responses, determine its importance, measure its importance, rank variables based on their importance, and show the magnitude of relationships [15,16]. These properties can be provided by the most recent machine learning methods (MLM) such as SHAP (SHapley Additive exPlanations).

As the most recent developed EAI system, SHAP can improve model transparency and be considered for any MLM. While the typical AI systems only employ linear or nonlinear regression as the alternate methods, SHAP covers both crucial aspects of a data mining assessment: data visualization and model explainability [24–28]. However, a comprehensive MLM will be required to construct a robust *CL* system and develop an accurate SHAP value assessment. For the first time, this work is going to implement the application of SHAP coupled with extreme gradient boosting (XGBoost) modeling (SHAP-XGBoost) through the mineral processing sector. XGBoost could do parallel processing, handling missing values, regularizing, pruning a non-greedy tree, and setting an objective function dynamically [29–33]. This investigation will develop a *CL* for a CF circuit in the Tabas Parvadeh coal plant using the SHAP-XGBoost model as a novel approach. For verification purposes, Pearson correlation, Random Forest, and support vector regression, as typical statistical and prediction tools, were also implemented through the dataset for comparing and assessing the SHAP-XGBoost capability.

2. Materials and methods

2.1. Column flotation circuit

Tabas Parvadeh coal plant is located in the central part of Iran. Its flotation circuit consists of 6 FCs ($D \times H$: 4.3 m × 8 m). In general, the plant is treated around 300 t/h coal ore containing 35%–55% ash to produce a concentrate with less than 11% ash. The feed is screened initially to make different size fractions, coarse (+6–50 mm), intermediate (+0.5–6 mm), and fine (−0.5 mm). The heavy medium circuits of Tri-Flo separators process coarse and intermediate size fractions. The fine fraction is transferred to the flotation circuit. Five columns (A, B, C, E, and F) were installed for the washing of −0.5 mm raw coal, and the other column (D) is used for cleaning the fine coal (−45 μm) stream obtained in dewatering centrifuges (Fig. 1). The fuel oil (as a collector) and MIBC (as frother) are added to the conditioning tank and feed distributor vessel, respectively. The flotation reagents were automatically added to the control room process by the operator orders and recorded. In the process, the washing water (water added via pans from the top of column flotation and used for washing the froth) was approximately as much water as reporting to the froth. Sensors measured froth level, and the specific gravity was determined by sampling from the feed. The dataset was collected from the plant for around one year (from 17 April 2016 to 10 March 2017). Variables from the whole CF circuit were recorded per shift (2 shifts per day) (Table 1). The representative metallurgical responses have been calculated as follows (f, c, and t are the ash content in the feed, concentrate, and tail (all in percent), respectively):

$$\text{Yield }(\%) = \frac{f-t}{c-t} \times 100 \tag{1}$$

$$\text{Separation Efficiency }(\%) = \frac{100c(f-t)}{f(c-t)} \tag{2}$$

2.2. SHAP

Lundberg and Lee [24] proposed the SHapley Additive exPlanations (SHAP) value as an essential tool for developing any EAI model. SHAP value is the average of the marginal contributions across all permutations (a novel methodology for explaining any MLM outputs). Typical variable importance assessments (such as Pearson correlation) only determine the relationship across the entire population but not on each individual case [25,26]. SHAP could tackle this drawback by providing local interpretability, which determines and contrasts the impacts of the factors. SHAP values (Φ_i) can be calculated based on Eq. (3). Where N is the set of all variables, and S is a subset of N. The models $V(S \cup \{x_i\})$ and $V(S)$ are trained with and without input variables, respectively. The predicted outputs of these two models were compared on the subset S current input [34,35].

$$\Phi_i = \sum_{S \subseteq N\{\{x_i\}} \left(\frac{|S|!(|N|-|S|-1)!}{|N|!} \right) [V(S \cup \{x_i\}) - V(S)] \tag{3}$$

According to this interpretation, the SHAP value for each individual variable could be determined, and the input parameters could be ranked based on their Φ_i. In the ranking diagram, the horizontal position of a variable indicates whether its impact is important for the prediction or not. The color would represent the correlation magnitude for that observation: positive (red) and negative (blue) [34,35].

2.3. XGBoost

Extreme gradient boosting (XGBoost) has shown exceptional accuracy and significant prediction exactness. Chen and Guestrin [36] developed XGBoost as an ensemble algorithm based on gradient boosted trees which has a powerful supervised learning system. It comprises several decision trees and uses the first-order and the second-order Taylor expansion of the loss function [37]. To avoid overfitting, XGBoost adds a regularization term utilized in the objective function and helps to reduce the model complexity. In other words, parallel and distributed computing leads to speed up the learning process. For controlling the model complexity through the generation of the m^{th} tree, the objective function in the m^{th} tree of the k^{th} category developed by:

$$\text{Obj}_{km} = L_{km} + \lambda_1 T_{km} + \frac{1}{2}\sum_{j=1}^{T_{km}} \left(\gamma_{jkm}^2\right) \tag{4}$$

where λ_1 is the coefficient of the number of leaf nodes; and T_{km} the number of leaf nodes in the first m trees or in the m^{th} trees [29–36,38].

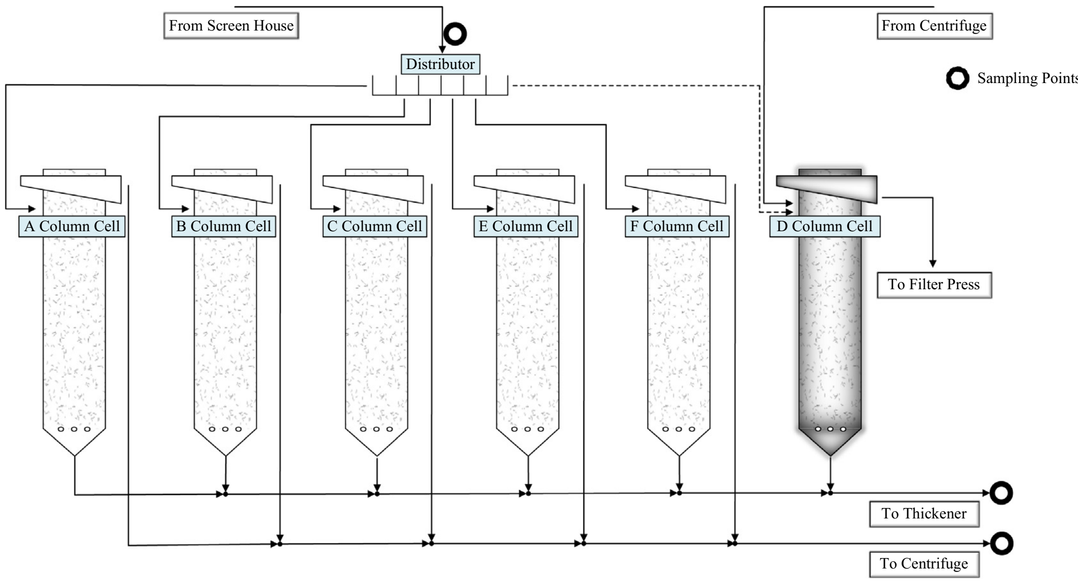

Fig. 1. Schematic of flotation column circuit in the Tabas Parvadeh coal plant.

Table 1
Operating variables and their representative metallurgical responses in the column flotation circuit.

Variables	Minimum	Maximum	Mean	Standard deviation
Solid percentage (%)	4.60	15.90	9.47	2.63
Frother dosage (L/h)	1.50	12.50	5.14	2.54
Collector dosage (L/h)	23.80	118.43	64.55	19.54
Airflow rate (dm^3/s)	28.60	41.00	36.39	3.24
Washing water (m^3/s)	0.00	30.20	16.13	8.67
Froth level (cm)	22.00	83.25	28.14	7.98
Specific gravity (SG)	1.65	1.75	1.72	0.04
Yield (%)	10.77	62.08	37.27	11.02
Separation efficiency (SE) (%)	12.99	61.04	43.83	8.30

2.4. Random Forest

Random Forest (RF) as a high-dimensional and non-parametric tree-based predictive model has been developed by Breiman [39]. RF is an ensemble MLM that chains many decision trees by taking the same number of bootstrap records from the main dataset, randomized subset of variables, and generating a tree-based for each bootstrap sample. The procedure of generating forest and bootstrap data can be described as a bagging technique. Through the bagging process, for developing a new training set for each tree, some records do not consider in the training of that tree that called out-of-bag (OOB) samples. A specific instance of OOB would increase the RF accuracy compared to other supervised MLM [40–43]. OOB randomly selects a bootstrapped record $\Gamma(\theta)$ of size n from the training set (Γ) of size N as the modified training set for each new tree. Each tree predictor $T_{\Gamma(\theta)}$ is dependent on the random vector θ, which shows the bagged samples from the main learning set Γ. The prediction f is the average values (with y'_η the predicted response for sample X_η, where k is the size of the ensemble) [42,44,45]:

$$y'_\eta = f(X_\eta) = \frac{1}{K}\sum_{k=1}^{k}\left(T_{\Gamma(\theta_k)}(X_\eta)_1^k\right) \tag{5}$$

2.5. Support vector regression

Support vector regression (SVR) is a powerful learning MLM with high generalization regression capability that reduces overfitting problems in the training phase. SVR as a novel AI system uses a promising nonlinear kernel-based regression method for minimizing the structural risk principle in high dimensional feature space [46,47]. In other words, SVR converts complex nonlinear regression problems into linear regression models by utilizing convex optimization techniques. This conversion develops an adjustment between the empirical error and the model complexity, leading to high prediction accuracy. In the SVR linear function f used to formulate the nonlinear relationship between X_i and Y_i:

$$f(x) = w\varphi(x) + b \tag{6}$$

$f(x)$ shows the predicted value, and the two parameters $w \in \Re^{n_h}$ and $b \in \Re$ must be adjusted. For structural risk minimization, empirical risk Eq. (7) can be considered where ξ (ξ-insensitive) is a precision parameter representing the radius of the tube located around the regression function [46,48,49].

$$\min R_e(w, \xi^*, \xi) = \frac{1}{2}|w|^2 + C\sum_{i=1}^{n}(\xi^* + \xi) \tag{7}$$

with these constraints:

$$\begin{cases} y_i - w\varphi(x_i) - b \leqslant \varepsilon + \xi_i, & i = 1,2,3,\cdots \\ -y_i + w\varphi(x_i) + b \leqslant \varepsilon + \xi_i, & i = 1,2,3,\cdots \end{cases}$$
$$\begin{cases} \xi_i^* \geqslant 0, & i = 1,2,3,\cdots \\ \xi_i \geqslant 0, & i = 1,2,3,\cdots \end{cases} \tag{8}$$

2.6. Models evaluation

Pearson correlation "r", coefficient of determination "R^2" and root mean square error "RMSE" were used to assess the models' outcome reliability. "r" linearly and singularly measures intercorrelations among all variables and rank it from −1 to +1. The sign of the r-value represents the relationship magnitude, and its absolute value demonstrates the correlation strength [50,51]. R^2, known as the "goodness of fit", was used to evaluate models' accuracy. R^2 ranges from 0 to 1 (R^2 closer to 1 represents high model reliability). In general, R^2 is the proportion of the variance in the output that is predictable from the input variables [52]. RMSE measures the differences between the predicted values by a model and the actual value (predicted values $\hat{y}_t$ for times t of a regression's dependent variable y_t):

$$\mathrm{RMSE} = \sqrt{\frac{\sum_{i=t}^{T} (\hat{y}_t - y_t)^2}{T}} \tag{9}$$

The "xgboost" and "shap" packages in Python, were used to develop the XGBoost and SHAP models. Moreover, Scikit-learn, a Python machine learning library, was employed to implement Random Forest and support vector regression.

3. Results and discussion

3.1. Relationship assessments

Exploring relationships for developing variable importance assessments to build a powerful *CL* were conducted by SHAP analyses through the whole dataset. SHAP analyses (Fig. 2) indicated that washing water within all the variables in the dataset had the highest importance for the yield prediction while the froth level had the lowest rank of importance. In other words, the washing water showed a significant impact on yield within the plant operating conditions. SHAP results illustrated that this impact is meaningful negative. In a CF, the addition of wash water provides the water necessary for the overflow of the collected solids into the launder. It increases froth stability and consents a deep froth bed to develop. Moreover, through the cleaning zone, the raised froth from the col-

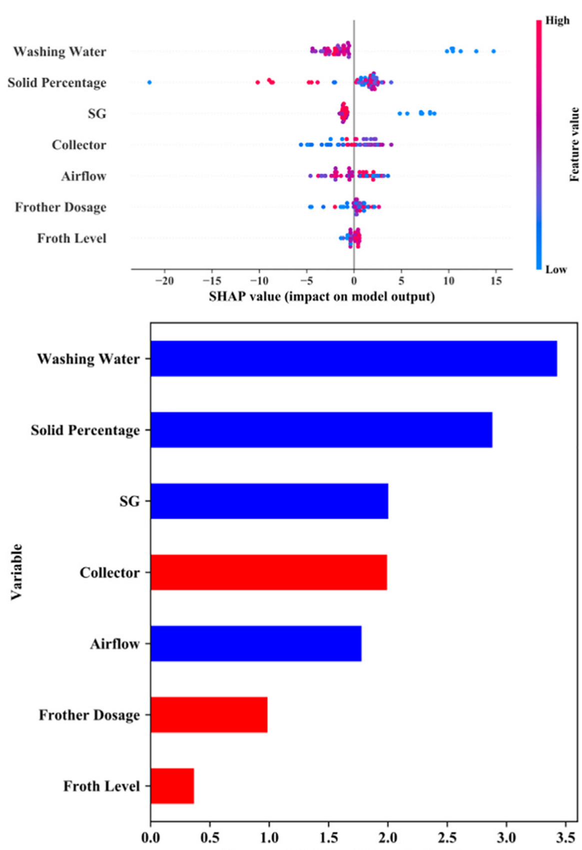

Fig. 2. SHAP analysis of variables for the yield prediction in the circuit.

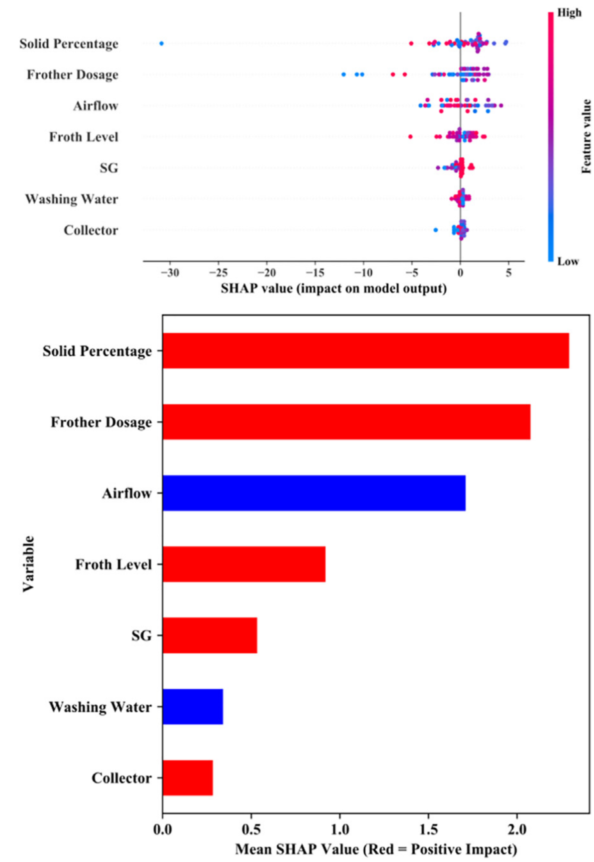

Fig. 3. SHAP analysis of variables for the separation efficiency prediction in the circuit.

Fig. 4. Pearson correlation between CF operational parameters and their metallurgical responses.

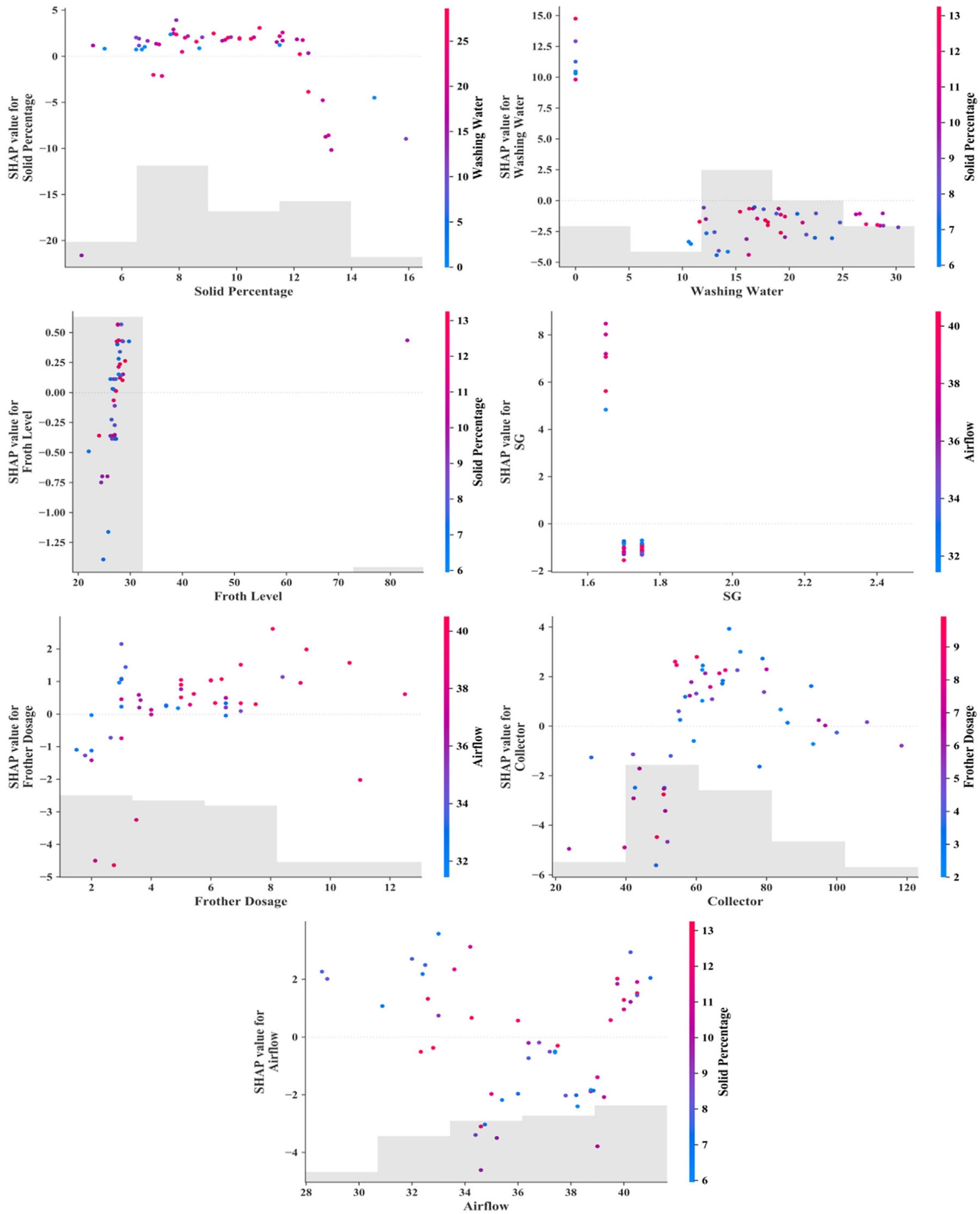

Fig. 5. SHAP multivariable correlation assessments among CF operating variables when yield was the target.

lection zone would be washed by counter-current water to remove the entrained gangue introduced at the top of the column [5]. In other words, without washing, the CF would not be able to attain the grade [6]. Thus, the yield would be decreased when the washing water was increased. It was reported that wash water rate has a slow impact on the interface level, bias rate, air holdup, and recovery but immediately affects the grade [23,53,54].

For the separation efficiency (SE), the solid percentage indicated the highest positive effect, where the collector concentration had the lowest importance with the plant operating conditions (Fig. 3). It was documented that due to the efficient cleaning action and the positive bias, a high solids percent feed can be subjected to a CF without destroying the concentrate grade. However, after a specific value, it has a negative effect on the recovery [6,55–57]. SHAP outcomes showed a significant negative correlation between solid percentages and yield (Fig. 2). Frother concentration depicted a positive correlation with both yield and SE. Frother addition to a certain level could reduce bubble size and bubble rise velocity and improve holdup [6]. A significant inter-correlation occurs among CF operating variables as froth level and airflow and washing water

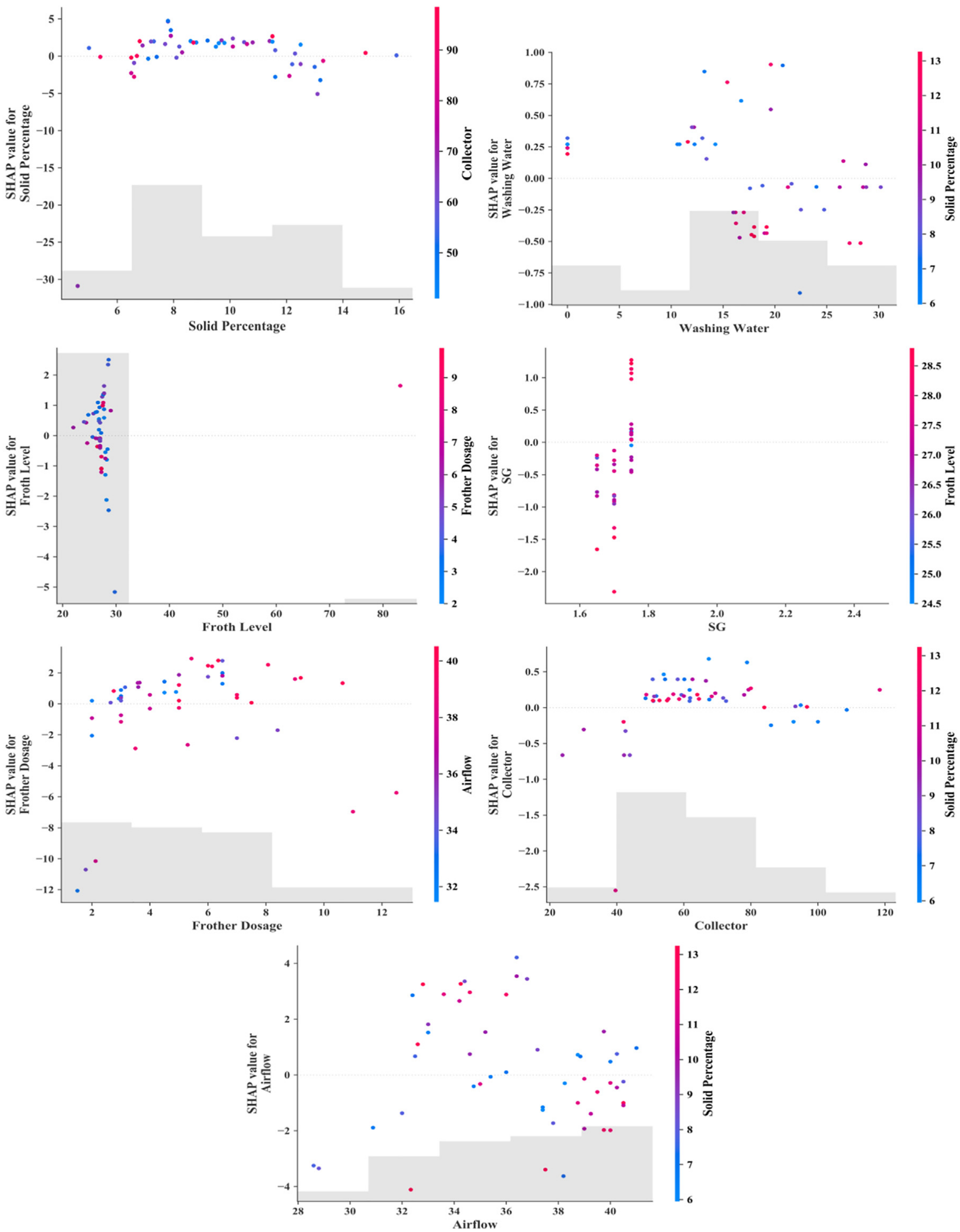

Fig. 6. SHAP multivariable correlation assessments among CF operating variables when separation efficiency was the target.

flow rates [53,54] that SHAP considered for determining relationships. In general, there is a good agreement between these results and Pearson correlation assessments (Fig. 4). However, SHAP assessed both linear and nonlinear multivariable relationships and plotted SHAP values for each sample that could be resulted in rank variables (Figs. 5 and 6). In contrast, Pearson correlation only considers a single linear relationship between two features and plots records' effect on the output.

Since one of the main parameters in a CF circuit is to keep the froth level [23] to have steady-state conditions through the operation, froth depth may have no significant effect on metallurgical responses [5,6]. However, a positive correlation has been reported between grade and froth height [22,23]. SHAP values determined a positive relationship between coal metallurgical responses and froth level within its variation in the dataset (Figs. 2 and 3). The airflow rate could cause a quick variation on froth level and air holdup, but a slow impact on bias and a medium variation on grade and recovery [23]. However, bubble size generated is a function of airflow rate, and SHAP values showed a negative relationship between airflow rate and coal metallurgical responses (Figs. 2

Table 2
The XGBoost parameter settings.

Parameter	Value (yield)	Value (SE)
Base learner	Gradient boosted tree	Gradient boosted tree
Tree construction algorithm	Exact greedy	Exact greedy
Learning objective	Regression with squared loss	Regression with squared loss
Learning rate (η)	0.725	0.607
Lagrange multiplier (γ)	9	6.5
Number of boosted trees	10	15
Maximum depth of trees	6	6
Minimum sum of weights	1	1

Table 3
Accuracy measures provided by the various examined machine learning methods in the testing phase.

Method	Yield		SE	
	R-squared	RMSE	R-squared	RMSE
Random Forest	0.87	3.99	0.54	3.98
Support vector regression	0.85	4.30	0.53	7.26
XGBoost	0.96	2.12	0.88	2.04

and 3). Outcomes showed a negative correlation between SG and the coal CF circuit's metallurgical responses reported in other investigations as well [4]. This negative relationship could be due to the high relationship between SG and ash in the coal content (by increasing the ash content, the SG of coal samples increased) [58]. SHAP values confirmed this negative correlation between SG and yield (Fig. 2). Within the dataset, collector concentration showed a medium positive effect on the coal metallurgical responses (Figs. 2 and 3).

3.2. Metallurgical responses' prediction

For developing XGBoost models to predict the CF metallurgical responses, from the whole dataset (51 recorded samples), 80% of records were randomly considered for the training set, and the rest of the data was used for the model's testing phase. The four main XGBoost hyperparameters are general, booster, learning task, and command-line parameters. General parameters are the overall functioning of the XGBoost model and include booster, verbosity, and nthread. From booster parameters, gbtree, gblinear, or dart can be selected. The verbosity of printing messages could be 0 (silent), 1 (warning), 2 (info), 3 (debug). The nthread can be used for parallel processing. The number of cores in the system has to be entered. The value should not be entered for running on all cores, and the algorithm would detect automatically. Tree and linear boosters are the XGBoost booster parameters. Tree booster typically outperforms the linear booster. Learning task parameters corresponded to the learning objective and define the optimization objective that needs to be calculated for the metric at each step. In this work, the hyperparameters were considered mainly the default of its algorithm. After the tuning process (a try and error procedure), the optimum model features are adjusted and applied for training (Table 2). The XGBoost results (Table 3) indicated that this MLM could accurately estimate the CF metallurgical responses based on the monitored operational variables. For comparison purposes, the same training and testing sets were considered to develop RF and SVR models. Results (Table 3) indicated that the XGBoost model provided significantly higher accuracy for predicting the CF metallurgical responses than these two known MLM (Fig. 7). These results depicted that SHAP-XGBoost could successfully develop a *CL* for the CF circuit as a powerful EAI system. These comprehensive outcomes could potentially be applied for modeling, controlling, and maintaining various processes on an industrial scale.

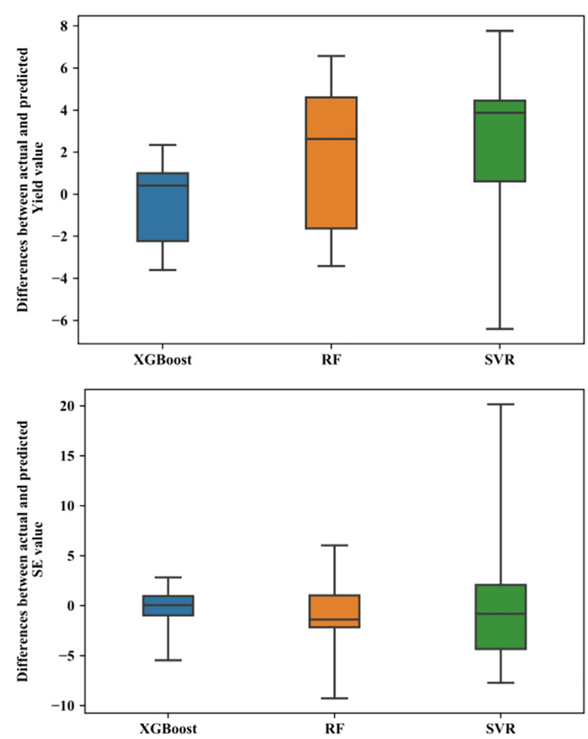

Fig. 7. Differences between actual and predicted coal metallurgical responses by different machine learning methods in the testing phase.

4. Conclusion

SHapley Additive exPlanations (SHAP) and extreme gradient boosting (XGBoost) for the first time have been used as an explainable artificial intelligence tool to develop a conscious-lab (*CL*). The generated *CL* was considered to assess and model relationships between operational variables and their representative metallurgical responses (yield and separation efficiency "SE") for an industrial coal column flotation circuit.

(1) SHAP could provide robust multivariable correlations among all the monitored variables and for each record of them. In general, SHAP values demonstrated that solid percentage and washing water have the highest effect on separation efficiency and yield, respectively.
(2) SHAP indicated the magnitude of relationships for all variables and records. An increase in the solid percentage could improve the separation efficiency of the column flotation unit, while increasing the washing water would decrease yield.
(3) XGBoost coupled with SHAP could provide a substantial prediction for the coal column flotation metallurgical responses. The coefficient of determination of the predictive model for the yield and separation efficiency was 0.98 and 0.88, respectively.
(4) The prediction accuracy of XGBoost-SHAP (root mean square error less than 2.2) was higher than Random Forest (root mean square error > 3.98) and support vector regression (root mean square error > 4.30)
(5) The SHAP-XGBoost outcomes suggested that the generated method could be successfully considered a *CL* for deep understanding and modeling industrial datasets.

Appendix A. Modeling of Ash reduction

See Fig. A1, Fig. A2, Fig. A3.

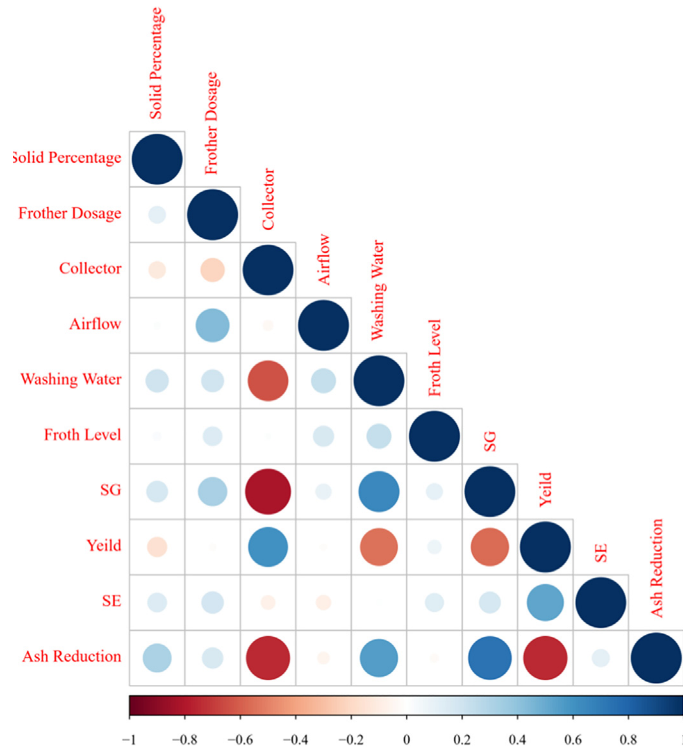

Fig. A2. Pearson correlations between Ash reduction and flotation variables.

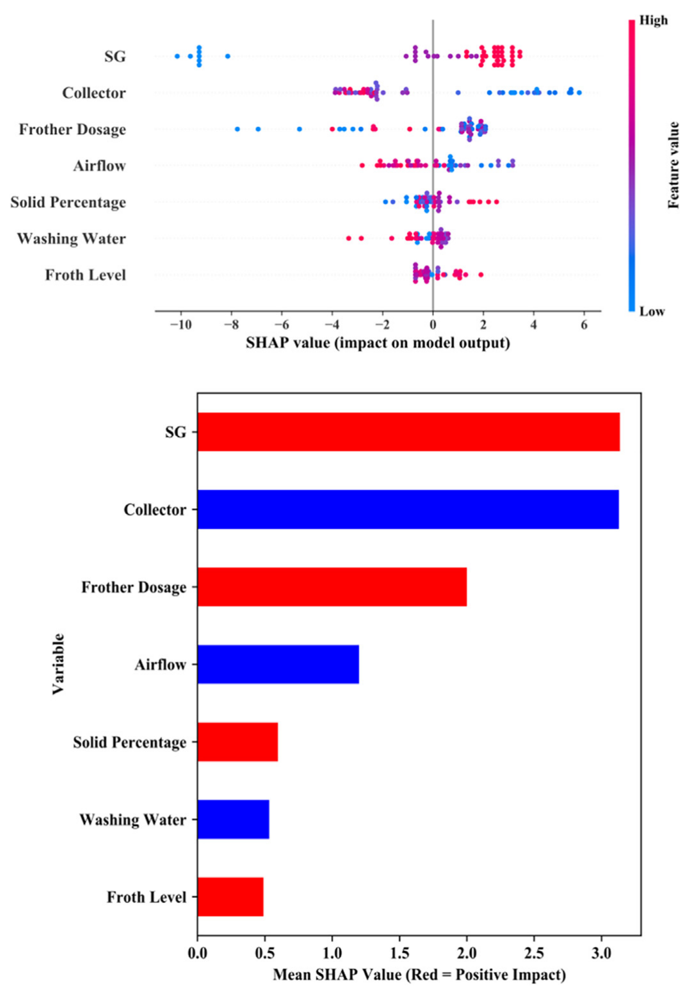

Fig. A1. Relationship between Ash reduction (as metallurgical response) and column flotation variables.

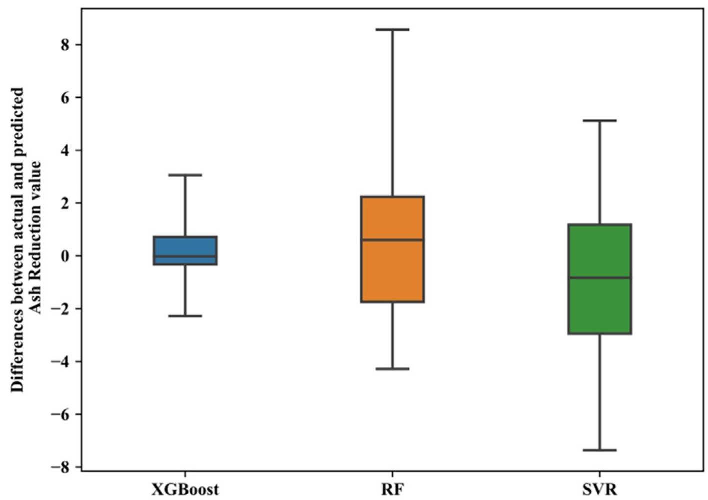

Fig. A3. Differences between actual and predicted values based on various models.

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