

Harnessing Machine Learning Models to Predict Flow Regimes over Stepped Spillways

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ABSTRACT

Accurate identification of flow regimes is crucial for understanding and analyzing flow behavior over stepped spillways. This study evaluates the ability of three machine learning regression models, namely AdaBoost Regressor (AdaBoost), Extra Trees Regressor (ETR), and Extreme Gradient Boosting (XGBoost), to predict three flow regimes (nappe flow, transition flow, and skimming flow) over stepped spillways. A dataset of 126 samples, including the ratio of critical flow depth to step height (h_c/h), chute slope (α), and flow condition, was collected from a hydraulic experimental study. Two data splitting ratios were used for model training and testing: 110:16 and 84:42. The models were evaluated and compared using Mean Absolute Error (MAE), Root Mean Squared Error (RMSE), coefficient of determination (R^2), and Overall Index (OI). The findings revealed that AdaBoost, ETR, and XGBoost achieved higher accuracy than previous studies that employed Artificial Neural Networks (ANNs) and the Adaptive Neuro-Fuzzy Inference System (ANFIS), with R^2 and OI exceeding 0.90 for both data-splitting ratios. The AdaBoost model demonstrated the highest performance, followed by ETR and XGBoost, respectively. This study contributes to the advancement of knowledge of machine learning models, particularly in their application to hydraulic engineering contexts.

Keywords-adaboost; extra trees; flow regimes; stepped spillways; XGBoost

I. INTRODUCTION

In hydraulic engineering, one of the most significant issues is the downstream scour phenomenon in hydraulic structures, which is caused by a large amount of flow kinetic energy [1-4]. To dissipate this energy at the toe and prevent downstream hydraulic structure scour, a hydraulic structure with steps from the crest to the toe - a stepped chute, stepped channel, or

stepped spillway - is used [5-9]. Moreover, the construction cost of the downstream stilling basin at the spillway's end can also be decreased by this hydraulic structure's optimal design [10, 11]. These stepped hydraulic structures are frequently utilized for storm waterways, irrigation channels, gabion weirs, and gabion spillways [12, 13]. They can also aid in the enhancement of atmospheric gas (nitrogen, oxygen) and volatile organic component air-water transport, which is

advantageous for water treatment facilities and in-stream re-aeration. Stepped hydraulic structures have been the subject of numerous research studies in a variety of areas. A precise prediction of the flow regime on the stepped hydraulic structures is crucial to understanding the hydraulic behavior along the spillway, including air entrainment [14, 15], cavitation [16], and energy dissipation [5, 8].

Recently, machine learning models have been successfully applied to address challenges in water science and engineering, including water quality monitoring and prediction [17-20], water treatment and management [21, 22], hydrological forecasting and runoff modeling [23-25], groundwater prediction [26, 27], and reservoir operations [28-31]. In the context of stepped spillways, machine learning models have been effectively applied to analyze energy dissipation [32-34], optimize spillway design [35], select spillway types [36], and interpret spillway performance [37]. However, when it comes to indicating flow regimes over stepped spillways, only two studies have utilized machine learning models: Artificial Neural Networks (ANNs) [38] and Adaptive Neuro-Fuzzy Inference System (ANFIS) [39]. To expand on this, this study investigates four additional machine learning models, namely Decision Tree Regressor (DTR), AdaBoost Regressor (AdaBoost), Extra Trees Regressor (ET), and Extreme Gradient Boosting (XGBoost), to examine flow regimes over stepped spillways.

II. FLOW CHARACTERISTICS OVER STEPPED SPILLWAYS

Based on several experimental hydraulic studies, stepped spillways can be classified as napped flow, transition flow, or skimming flow [7, 9]. During low discharge, a napped flow mechanism takes place, causing the flow to leave the upper step and descend. The skimming flow regime occurs when the discharge is high. For this flow regime, water is trapped between the steps and a virtual boundary forms between the flow and steps. Additionally, the transition regime is a flow state that exists between the skimming and napped regimes.

A. Nappe Flow Regime

A series of free-falling jets with nappe impact on the downstream step behaves for low-flowing discharge on a flat-step geometry. At the upstream end of each step, an air cavity and a pool of recirculating fluid are defined. Additionally, the air is entrained at the jet interfaces and via a plunging jet mechanism at the lower nappe's intersection with the recirculating pool, although de-aeration is frequently observed downstream. Interfacial aeration occurs at both the upper and lower nappes of the free-falling nappe. The shear layer that forms in the lower nappe is characterized by high turbulence and significant interfacial air entrainment [40, 41].

B. Transition Flow Regime

The concept of a transition flow regime was introduced in [42]. A variety of flow rates for a given stepped-channel chute shape produces an intermediate flow regime between nappe flows at low discharges and skimming flows at high discharges. Air bubble entrainment occurs in the spray region downstream of the stagnation point and along the jet upper

nappe in the transition flow regime. There is constant mixing of water and air in this extremely turbulent flow, and there is still much to learn about the air entrainment process in the transition flow.

C. Skimming Flow Regime

In stepped spillways, the skimming flow regime typically occurs at high discharge rates when the relative step height (the ratio of the step height to the critical depth) becomes small. This flow regime is considered two-dimensional and is advantageous for nonintrusive flow visualization techniques [40-44]. The steps' external edges produce a pseudo-bottom, which the flow skims over. Recirculating vortices arise under the pseudobottom. Recirculation is maintained by the transmission of shear stress from the main stream. At the corner of the steps, small-scale vorticity is also formed. The aerated flow region follows a region with a smooth, glassy-free surface. Turbulence forms near the boundary. Furthermore, the boundary layer increases until the outside edge of the boundary layer touches the surface. Turbulence can trigger natural free-surface aeration when the boundary layer's outer edge reaches the free surface. The point of inception is the location where air entrainment begins. The flow becomes rapidly aerated downstream of the origin point of the free surface aeration and the free surface appears white. By thoroughly mixing air and water, a two-phase homogeneous flow is created.

III. MACHINE LEARNING MODELS AND THEIR APPLICATION IN HYDROINFORMATICS

A. AdaBoost Regressor (AdaBoost)

AdaBoost [45] combines multiple weak learners, typically decision trees, to create a robust predictive model. Its iterative re-weighting mechanism gives tough samples more weight, which makes it effective at dealing with nonlinear and high-dimensional data. Adaboost initially gives all samples equal weights, which are adjusted iteratively based on prediction errors.

$$\hat{y}(x) = \sum_{m=0}^M \alpha_m h_m(x) \quad (1)$$

where $\alpha_m = \frac{1}{2} \ln\left(\frac{1-e_m}{e_m}\right)$ is the weight of the m -th weak learner and e_m is its error. Sample weights are updated iteratively to emphasize misclassified samples:

$$w_i^{(m+1)} = w_i^m \exp(\alpha_m \cdot \mathbb{1}(y_i \neq \hat{y}_i)) \quad (2)$$

B. Extra Trees Regressor (ETR)

ETR, also known as extremely randomized trees, is an ensemble learning method that consists of four steps:

1. Randomized splitting: Unlike traditional decision trees, ETR selects split points randomly. At each node, a subset of features is randomly chosen and each feature at random selects a split threshold from its value range. This randomization reduces the correlation between trees and reduces the risk of overfitting.
2. Tree construction: ETR builds trees independently without bootstrapping the data, unlike Random Forests (RF). Each tree is trained on the entire dataset, enhancing tree diversity [46].

3. Leaf node predictions: For regression tasks, each tree predicts a numerical value at the leaf node, which is the average of the target values for all samples falling in that leaf.
4. Ensemble averaging: The final prediction is the average of the predictions from all trees.

$$\hat{y}(x) = \frac{1}{T} \sum_{t=1}^T h_t(x) \quad (3)$$

where T is the total number of trees in the ensemble, and $h_t(x)$ is the prediction of the t -th tree for input x .

C. Extreme Gradient Boosting (XGBoost)

XGBoost is a gradient-boosting algorithm optimized for speed and accuracy. Its ability to model non-linear relationships, handle missing values, and evaluate feature importance is crucial for hydrological datasets. XGBoost builds on gradient boosting by adding regularization to enhance generalization and incorporating optimizations for speed and efficiency. The objective function includes a loss term and a regularization term:

$$\mathcal{L} = \sum_{i=1}^n l(y_i, \hat{y}_i) + \sum_{k=1}^K \Omega(f_k) \quad (4)$$

where n is the number of data points in the dataset, $l(y_i, \hat{y}_i)$ is the loss function for data point i , such as squared error $l(y_i, \hat{y}_i)^2$, K is the number of trees in the model, and $\Omega(f_k)$ is the regularization term for the k -th tree, defined as:

$$\Omega(f_k) = \gamma T_k + \frac{1}{2} \lambda \|w\|^2 \quad (5)$$

where γ is a parameter that controls tree complexity by penalizing the number of leaves, T_k denotes the number of leaves in the k -th tree, λ is a parameter that controls the penalty on the L2 norm of the leaf weights w , and w is the vector of leaf weights for the k -th tree.

IV. MODEL DEVELOPMENT AND EVALUATION

Figure 1 displays the overall procedures and frameworks in this study. The details can be elaborated as follows.

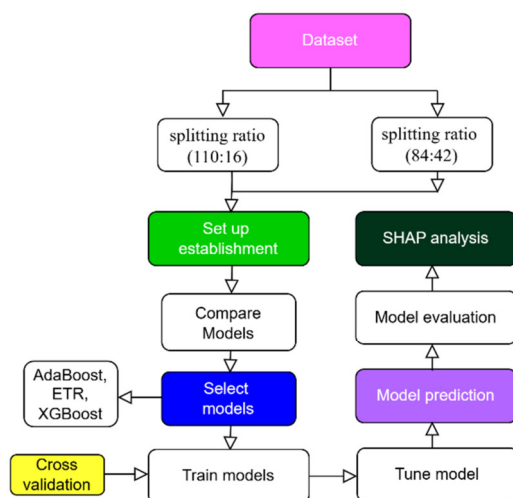


Fig. 1. Overall procedures and frameworks.

A. Data Used and Preprocessing

For the experiment, 126 samples were collected from previous studies to predict the flow regime in stepped channels using ANNs with multi-layer backpropagation networks [38] and ANFIS [39]. These studies utilized data collected from hydraulic laboratory tests to examine the aeration performance in stepped spillways at the Civil Engineering Department of Firat University in Elazig, Turkey [47, 48]. The steps were installed in a prismatic rectangular chute with dimensions of 0.30 m in width and 0.50 m in depth. Transparent methacrylate was used for the side walls to observe flow conditions. Pumped from the storage tank to the stilling tank, water entered the chute through an approach channel with a bed that was 1.25 and 2.50 m above the laboratory floor. A downstream channel with dimensions of 3.0 m in length, 0.35 m in width, and 0.45 m in depth was used for this investigation. Unit discharges, measured using a flow meter installed in the supply line, ranging from 16.67×10^{-3} to 166.67×10^{-3} m²/s, were used in the experiments. For all slopes tested, equal to 14.48°, 18.74°, 22.55°, 30°, 40°, and 50°, step heights of 5, 10, and 15 cm were used.

The 126 samples were split into two groups: 110 for training and 16 for testing [38], and 84 for training and 42 for testing [39]. The performance of the models was evaluated using these two different training and testing splits. Table I describes the characteristics of the dataset. The parameters considered in this study include the ratio of critical flow depth to step height (h_c/h), chute slope (α), and flow regime. The first two parameters (h_c/h and α) serve as inputs to the models for predicting the flow regime. The three flow regimes, nappe, transition, and skimming, are represented by the numbers 1, 2, and 3, respectively. For the first split ratio, the training set contained 39 nappe, 26 transition, and 45 skimming cases, while the testing set included 7, 1, and 8 cases, respectively. For the second split ratio, the training set comprised 30 nappe, 19 transition, and 35 skimming cases, whereas the testing set consisted of 16, 8, and 18 cases, respectively.

B. Setup and Model Creation

This study used the PyCaret automated machine learning package within the Colab Python environment to initialize the setup and develop models. The four top-performing machine learning models were then identified and selected for further investigation.

The setup function was initialized with mandatory features and target variables, providing both functional and object-oriented APIs. MAE was used as the criterion to select the top three models from the 25 regression algorithms available in PyCaret. To enhance generalization and mitigate overfitting, a 10-fold Cross-Validation (CV) strategy with random splits was applied during model training [49], particularly given the small dataset size of 126 samples. Additionally, all selected models, AdaBoost, ETR, and XGBoost, incorporated regularization techniques, such as L1/L2 penalties, to prevent excessive model complexity by penalizing large weights [50]. The models were then fine-tuned using the 'tune model' function, optimizing their hyperparameters based on the lowest MAE value. A random search technique was employed for hyperparameter tuning, as it is more efficient than the

traditional grid search method [46, 51]. The tuned models were evaluated using the testing datasets to assess their predictive performance. Finally, the influence of each input variable on the model's predictions was analyzed using SHapley Additive exPlanations (SHAP).

TABLE I. STATISTICAL ANALYSIS OF USED DATA SETS

Data statistics	Training			Testing		
	h/h	alpha	Flow regime	h/h	alpha	Flow regime
Dataset splitting ratio (110:16) for training and testing						
Mean	1.01	29.42	2.05	1.07	28.42	2.06
Std	0.69	12.5	0.88	0.69	12.31	1
Min	0.2	14.48	1	0.32	14.48	1
Max	2.82	50	3	2.44	50	3
Dataset splitting ratio (84:42) for training and testing						
Mean	1.02	29.29	2.06	1.02	29.31	2.05
Std	0.69	12.57	0.88	0.7	12.3	0.91
Min	0.2	14.48	1	0.2	14.48	1
Max	2.82	50	3	2.82	50	3

C. Statistical Evaluation Matrices

Three machine learning models were investigated, and their performance was evaluated and compared with each other as well as with findings from the two previous studies using metrics such as Mean Absolute Error (MAE), Root Mean Squared Error (RMSE), coefficient of determination (R^2), and Overall Index (OI). When the values of OI and R^2 equal 1, it indicates a perfect match between the predicted and observed values. Conversely, for error terms, lower values demonstrate better model performance, indicating its ability to predict accurately.

1) Mean Absolute Error (MAE)

MAE is a widely used metric for regression problems. It measures the average magnitude of errors in a set of predictions without considering their direction. MAE is defined as:

$$MAE = \frac{1}{n} \sum_{i=1}^n |y_i - \hat{y}_i| \quad (6)$$

where y_i is the observed value, \hat{y}_i is the predicted value, and n is the total number of observations. MAE is simple to interpret as it retains the same unit as the target variable, making it intuitive for understanding prediction accuracy. However, it does not penalize larger errors more severely than smaller ones. In [52], the applicability of MAE in climate and environmental modeling was highlighted due to its robustness to outliers.

2) Root Mean Squared Error (RMSE)

RMSE is another popular metric that measures the square root of the average squared differences between observed and predicted values. It is expressed as:

$$RMSE = \sqrt{\frac{1}{n} \sum_{i=1}^n (y_i - \hat{y}_i)^2} \quad (7)$$

where y_i is the observed value, \hat{y}_i is the predicted value, and n is the total number of observations. RMSE penalizes larger errors more than MAE because it squares the residuals, making it sensitive to outliers. This property is both a strength and a limitation, depending on the use case. In [53], it was noted that RMSE is effective in applications where large errors are particularly undesirable, such as hydrological and meteorological forecasting.

3) Coefficient of Determination (R^2)

R^2 measures the proportion of variance in the dependent variable that is predictable from the independent variables and is calculated as:

$$R^2 = 1 - \frac{\sum_{i=1}^n (y_i - \hat{y}_i)^2}{\sum_{i=1}^n (y_i - \bar{y})^2} \quad (8)$$

where y_i is the observed value, \hat{y}_i is the predicted value, and n is the total number of observations. R^2 ranges from 0 to 1, with higher values indicating a better model fit. Negative values can occur when the model performs worse than the mean prediction. In [54], the importance of R^2 in linear regression was highlighted but it has limitations in non-linear models or when comparing models with differing numbers of predictors.

4) Overall Index (OI)

OI is a composite metric that evaluates model performance by combining various error metrics as:

$$OI = \frac{1}{2} \left[2 - \sqrt{\frac{\sum_{i=1}^n (y_i - \hat{y}_i)^2}{n}} - \frac{\sum_{i=1}^n (y_i - \hat{y}_i)^2}{y_{i,max} - y_{i,min}} - \frac{\sum_{i=1}^n (y_i - \hat{y}_i)^2}{\sum_{i=1}^n (y_i - \hat{y}_i)^2} \right] \quad (8)$$

where y_i is the observed value, \hat{y}_i is the predicted value, and n is the total number of observations. OI provides a single measure to assess model accuracy relative to the variability of the observed data. In [55], OI was introduced as part of model evaluation guidelines in hydrological simulations, emphasizing its usefulness in multi-objective evaluations.

V. RESULTS AND DISCUSSION

A. Model Performance Comparison

The model performance based on the first data split ratio (110:16) was evaluated as shown in Table II. AdaBoost achieved perfect performance with MAE and RMSE values of 0 and R^2 and OI values of 1, demonstrating its exceptional accuracy in predicting flow regimes over stepped spillways. ETR and ANNs, the latter taken from the previous study as a benchmark, also performed well, with ETR achieving an R^2 of 0.9983 and an OI of 0.9893, while ANNs achieved an R^2 of 0.9996 and an OI of 0.9953. However, both models had slightly higher MAE and RMSE values than AdaBoost. XGBoost, with an R^2 of 0.9332 and an OI of 0.9041, demonstrated the lowest accuracy among the models. Overall, AdaBoost emerged as the most effective model, significantly outperforming ANNs, which served as a benchmark, and highlighted the potential of ensemble-based machine learning models in hydraulic engineering applications.

TABLE II. MODEL PERFORMANCE FOR DATASET SPLITTING RATIO (110:16) FOR TRAINING AND TESTING

Models	MAE	RMSE	R ²	OI
AdaBoost	0.0000	0.0000	1.0000	1.0000
ETR	0.0137	0.0395	0.9983	0.9893
XGBoost	0.0628	0.2498	0.9332	0.9041
ANN	0.0131	0.0182	0.9996	0.9953

Model performance based on the second data split ratio (84:42) was evaluated and compared with ANFIS from the previous study, which served as a benchmark (see Table III). Among the models, AdaBoost achieved the best performance with an OI of 0.9786 and the lowest MAE (0.0497), although its RMSE (0.2184) and R² (0.9409) were slightly lower than ETR, which recorded an R² of 0.9405 and an OI of 0.9585. ANFIS demonstrated good predictive capability with an R² of 0.9483 and an OI of 0.9122 but had the highest MAE (0.1382) and RMSE (0.2044) among all models. XGBoost, while outperforming ANFIS in terms of MAE (0.0945) and RMSE (0.2905), exhibited the lowest R² (0.8954) and was less accurate than both AdaBoost and ETR. Overall, AdaBoost and ETR proved to be the most effective models for predicting flow regimes, significantly outperforming the ANFIS benchmark.

TABLE III. MODEL PERFORMANCE FOR DATASET SPLITTING RATIO (84:42) FOR TRAINING AND TESTING

Models	MAE	RMSE	R ²	OI
AdaBoost	0.0497	0.2184	0.9409	0.9786
ETR	0.0819	0.2192	0.9405	0.9585
XGBoost	0.0945	0.2905	0.8954	0.9490
ANFIS	0.1382	0.2044	0.9483	0.9122

Figure 2 presents a heatmap for error analysis across different flow regimes, highlighting the performance of various models. For the dataset split ratio of 110:16, the AdaBoost model demonstrated the highest reliability across all regimes, exhibiting the lowest error values. In contrast, XGBoost and ETR showed weaknesses in specific cases, particularly in the nappe and transition regimes, respectively. For the dataset split ratio of 84:42, both AdaBoost and XGBoost performed better overall, especially in the nappe regime. However, in the transition regime, all models exhibited relatively higher errors, indicating that predicting this regime is more challenging.

Ensemble methods such as AdaBoost and ETR make more practical sense for actual hydraulic monitoring systems since they do not need as much computing power and offer straightforward decision-making guidelines. Neural networks (ANNs) and neuro-fuzzy systems (ANFIS) are just not as feasible for field deployment because they are more computationally intensive and need specialists to fine-tune them properly [6].

B. Impact of Data Splitting Ratios on Model Generalization and Applications

The two data-splitting ratios (110:16 and 84:42) had noticeable effects on the predictive performance of the machine learning models. In the first ratio (110:16), where a larger portion of the data was allocated for training, models such as AdaBoost and ETR achieved near-perfect or highly accurate predictions, with R² and OI consistently above 0.99 and

minimal errors (MAE and RMSE close to zero). This highlights the advantage of having a more extensive training dataset, which allows models to learn intricate patterns and relationships within the data, resulting in superior predictive accuracy. Conversely, the second ratio (84:42), which allocated a larger portion of the dataset for testing, introduced greater variability in model performance. Although AdaBoost still demonstrated strong predictive capability, its performance slightly declined compared to the first ratio, with increased RMSE (0.2184) and a marginally lower R² (0.9409). Similarly, ETR, which was highly accurate in the first split, exhibited slightly reduced R² (0.9405) and higher errors. This suggests that the reduced training dataset in the second ratio may have limited the models' ability to generalize complex relationships effectively. These results highlight the importance of training dataset size in machine learning model performance. Larger training datasets (as in the 110:16 split) generally allow models to achieve better predictive accuracy, while smaller training datasets (as in the 84:42 split) can limit their performance due to reduced learning capacity. This underscores the need for careful consideration of data-splitting strategies when evaluating machine learning models, particularly for applications in hydraulic engineering where accuracy is critical.

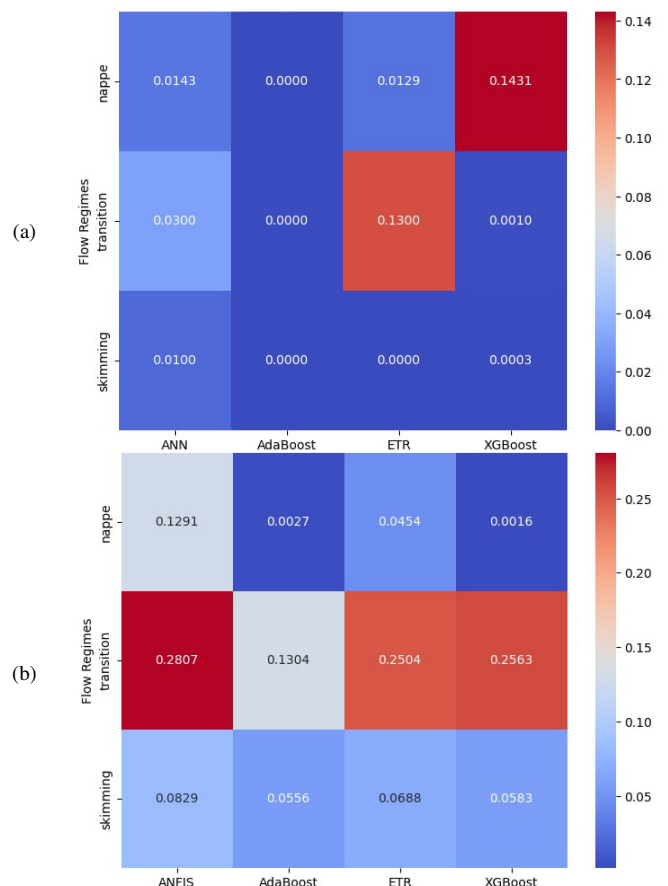


Fig. 2. Heatmap of model errors across different flow regimes: (a) split ratio (110:16), (b) split ratio (84:42).

C. Influence of Each Input Variable on Model Predictions

To evaluate the influence of each input variable on the model predictions, SHAP was applied after model training. SHAP is particularly effective for interpreting black-box models by explaining model behavior and quantifying feature contributions to individual predictions [56]. Figure 3 presents SHAP summary plots for two different data splitting ratios, illustrating the impact of input features on model predictions. In both cases, hc/h had the most significant influence, with lower values (blue) reducing the predictions and higher values (red) increasing them, and α (chute slope) has a secondary effect, although its impact distribution varies between the two graphs. The second graph shows a more stable and compact distribution of SHAP values, suggesting possible differences in dataset composition, model behavior, or feature interactions.

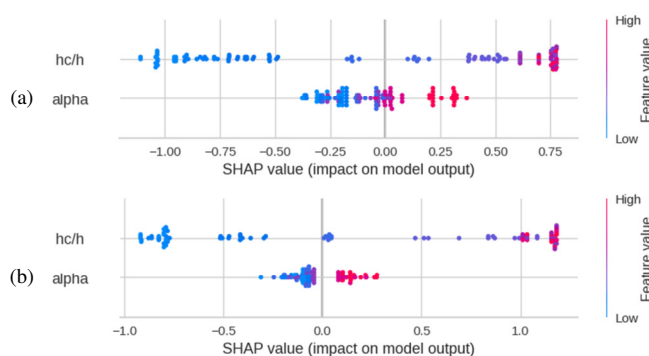


Fig. 3. SHAP plots illustrating the impact of the input features, (a) split ratio (110:16), (b) split ratio (84:42).

Future studies will involve additional hydraulic laboratory experiments to obtain larger datasets encompassing diverse flow conditions, thereby strengthening the reliability and applicability of the models to hydraulic engineering applications.

VI. CONCLUSIONS

This study presented a novel application of ensemble-based machine learning models to predict flow regimes over stepped spillways, demonstrating their superior performance compared to traditional approaches. Specifically, AdaBoost and ETR outperformed conventional models, such as ANNs and ANFIS, in terms of predictive accuracy and robustness. AdaBoost consistently delivered state-of-the-art performance, achieving near-perfect metrics (R^2 and OI exceeding 0.99 in the first split and 0.94 in the second split), while ETR also exhibited strong predictive capability. This study introduced a comparative evaluation of machine learning models in the context of hydraulic engineering, emphasizing the impact of data split ratios on model performance, a factor often overlooked in similar studies. The results indicate that larger training datasets enhance model accuracy, providing insight into optimal data utilization strategies for predictive modeling in hydraulic applications. By bridging the gap between traditional hydrodynamic modeling and advanced computational intelligence, this work contributes to the evolution of hydraulic structure analysis, offering more accurate, efficient, and

reliable tools for engineers and researchers. These findings not only reinforce the practical applicability of ensemble learning techniques in hydraulic engineering but also lay the groundwork for future studies integrating hybrid and deep learning models to further improve flow regime predictions in complex hydraulic systems.

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