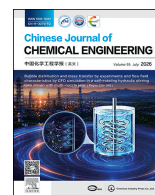




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Full Length Article

Interpretable machine learning-based prediction of hydrodynamic performance of divided fixed-valve tray in distillation columns

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ABSTRACT

Accurate prediction of tray hydrodynamics is essential for the design and optimization of modern distillation equipment. Conventional empirical correlations often show limited generalizability across diverse operating conditions, restricting their practical applicability. In this study, a data-driven modeling (DDM) framework integrated with Interpretable machine learning (ML) was developed to predict the hydrodynamic characteristics of a divided fixed-valve tray, including wet pressure drop, clear liquid height, weeping rate, and entrainment rate. A total of 760 experimental data points were obtained from cold-model experiments. Four machine learning algorithms—Random Forest, Extreme Gradient Boosting, Support Vector Regression, and a shallow Multilayer Perceptron—were trained and compared. Model performance was evaluated using the coefficient of determination (R^2), root mean square error (RMSE), and a composite R^2 -based index (R_{com}). Among these, the SVR model achieved the highest predictive accuracy, with R_{com} values of 0.9750 and 0.9834 for the test and extension sets, respectively. Building upon the best-performing SVR model, an expanded feature set was constructed using physically informed transformations of the orifice kinetic energy factor and overflow strength. Pearson correlation and SHAP analyses were applied to quantify each feature's contribution, revealing the dominant hydrodynamic drivers and clarifying their positive or negative influences on tray behavior. The integrated modeling and interpretability framework not only enhances predictive reliability but also provides actionable insight for guiding tray design and operational optimization.

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1. Introduction

Tray columns are essential equipment in distillation, absorption, and other separation processes, and have been extensively applied in chemical industries. Over several decades, numerous innovative tray designs have been developed to enhance mass transfer efficiency and gas-liquid interaction. Representative examples include the flow-guiding sieve tray [1], tridimensional rotational flow sieve tray [2–4], orthogonal wave tray [5], foam monolithic tray [6,7], Nye tray [8,9], spiral nozzle tray [10], vortex

tray [11,12], and total spray tray [13]. Accurate evaluation of the hydrodynamic performance of these emerging tray types is crucial for their structure optimization and industrial implementation.

Traditionally, the relationship between tray hydrodynamics and vapor-liquid loadings has been investigated using model-driven modeling (MDM) approaches based on physical laws, conservation equations, or theoretical correlations. For instance, Kotschering *et al.* [14] proposed an equivalent clear liquid height correlation for dualflow tray, which was later modified by Xu *et al.* [15] to accommodate larger tray diameters. Zhang *et al.* [16] further incorporated the effect of hole spacing to refine this model. In terms of entrainment, Kister and Haas [17] and Bennett *et al.* [18] developed empirical correlations for entrainment rate, while Uys *et al.* [19] experimentally demonstrated that liquid viscosity strongly affects entrainment—an effect not captured in earlier

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formulations. Zhang and Tan [20,21] proposed theoretical models for bubble formation and weep under static and cross-flow conditions. However, the actual multiphase flow behavior above tray perforations is highly complex and variable, making it difficult for conventional MDM approaches to capture such phenomena accurately. Developing a comprehensive theoretical model suitable for new tray configurations remains challenging. Distillation processes involve multiple interacting variables, such as gas-liquid properties, operating conditions, and tray geometry, which are often highly nonlinear. Furthermore, any structural modification or change in flow regime typically requires extensive experimental work to recalibrate or even re-derive the model parameters [22,23].

Against this background, data-driven modeling (DDM) provides a flexible and efficient alternative. Unlike physics-based approaches, DDM derives variable relationships directly from data without predefined mechanistic assumptions, making it particularly effective for nonlinear and multivariate systems [24]. As the core of DDM, machine learning (ML) techniques have been extensively adopted in chemical process modeling. Recent studies in chemical engineering have demonstrated the strong potential of ML-assisted DDM: Hu *et al.* [25] developed a hybrid framework that couples CFD with Bayesian optimization and large language models to efficiently explore multi-objective trade-offs in fixed-bed reactors, demonstrating the potential of data-driven strategies for intelligent reactor design. In a broader context, Zhu *et al.* [26] systematically reviewed machine-learning applications in multiphase hydrodynamics, transport, and reactions, highlighting how data-driven and physics-informed models can complement conventional CFD to improve prediction accuracy and accelerate process optimization. Wang *et al.* [27] developed an XGBoost-AdaBoost-ET ensemble framework and achieved enhanced predictive accuracy for nonlinear distillation modeling; Bi and Qiu [28] proposed a GA-PSO-optimized SVM for crude-oil property prediction and demonstrated superior performance compared with conventional SVM. Soroush *et al.* [29] employed a Levenberg-Marquardt ANN to model acid-gas absorption behavior with high regression fidelity, while Liu *et al.* [30] integrated CFD simulations with several ML algorithms and identified Gaussian Process Regression as the most reliable surrogate for reaction optimization. Xu *et al.* [31] introduced a chaos-wavelet neural network to predict pressure-drop signals in vapor-liquid-solid flow boiling with markedly improved accuracy; Zhou *et al.* [32] developed a hybrid CFD-LSTM model capable of predicting conversion and concentration profiles with orders-of-magnitude acceleration relative to CFD. Lahiri *et al.* [33] applied a GA-optimized SVR framework for slurry-flow pressure-drop prediction and reported significant improvements over empirical correlations; Chen *et al.* [34] compared multiple ML models for the volumetric mass transfer coefficient prediction in stirred bioreactors and identified CatBoost and XGBoost as the most suitable for Newtonian and non-Newtonian systems, respectively.

Compared with MDM and CFD simulations, ML-assisted DDM maintains high predictive accuracy while drastically reducing computational demands, particularly for complex or large-scale flow systems [32]. Although data-driven approaches have not been widely explored in tray hydrodynamics, their potential is increasingly recognized with the advancement of artificial intelligence. Once properly trained, DDMs can effectively replace empirical correlations and be seamlessly integrated into optimization frameworks. Therefore, this study systematically evaluates multiple ML algorithms to determine the most suitable DDM approach for predicting the hydrodynamic behavior of a divided fixed-valve tray. Furthermore, a hybrid framework combining DDM with interpretability ML is developed to identify the optimal

operating window and provide practical guidance for tray design and scale-up.

2. Methods

The workflow of this study is illustrated in Fig. 1. During the data acquisition phase, a divided fixed-valve tray was investigated. The orifice kinetic energy factor and overflow strength were selected as the input variables, whereas the wet pressure drop, clear liquid height, weep rate, and entrainment rate were defined as the output targets. An initial exploratory data analysis was conducted to examine data distributions and detect anomalies, followed by pre-processing to ensure data quality and consistency. The dataset was then randomly divided into training and testing subsets at a 4:1 ratio [35]. Various ML models were trained using the train set. Hyperparameter optimization was performed automatically using Optuna to identify the optimal parameter configuration for each model, thereby ensuring their best regression performance. A comprehensive evaluation metric (R_{com}) was formulated to compare the predictive accuracy and generalization capability of all models on the same test and extension sets. This comparison enabled the identification of the most suitable model for predicting tray hydrodynamic performance. We employed physically informed feature engineering on the selected model to disentangle the individual and interactive contributions of F_0 and L_W to the four hydrodynamic responses. The combined use of correlation analysis and SHAP establishes a transparent basis for identifying key drivers and guiding subsequent interpretation and optimization.

2.1. Experimental approach

The structure of the divided fixed-valve tray used in this study is depicted in Fig. 2. The tray valve consists of two components: a cap and three supporting legs. The cap includes a central disk ($\phi 20$ mm) with a 5 mm-wide peripheral flange bent downward, while the legs—arranged at 60° intervals—have a trapezoidal shape (upper base: 10 mm, lower base: 7 mm, height: 11 mm) and are connected to the flange at their slanted edges. The divided tray has 74 fixed valves with a spacing of 70 mm. The hydrodynamic performance of the divided tray was evaluated using a cold-flow experimental setup, schematically shown in Fig. 3. Experiments were carried out in a transparent acrylic column (height: 3.5 m, internal diameter: 796 mm). Water was employed as the liquid phase. It was pumped from a tank into the top of the column *via* a centrifugal pump. After flowing across the tray, the liquid

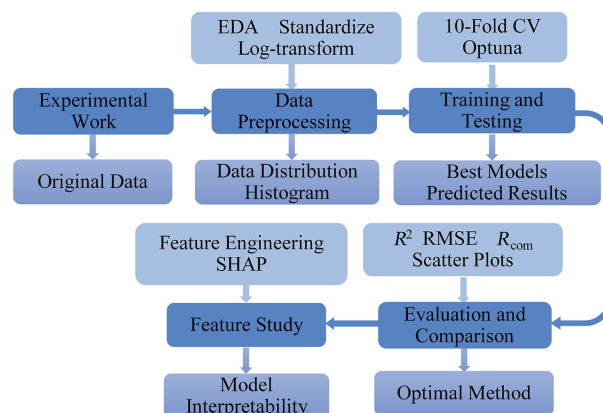


Fig. 1. Illustration of the workflow for the research.

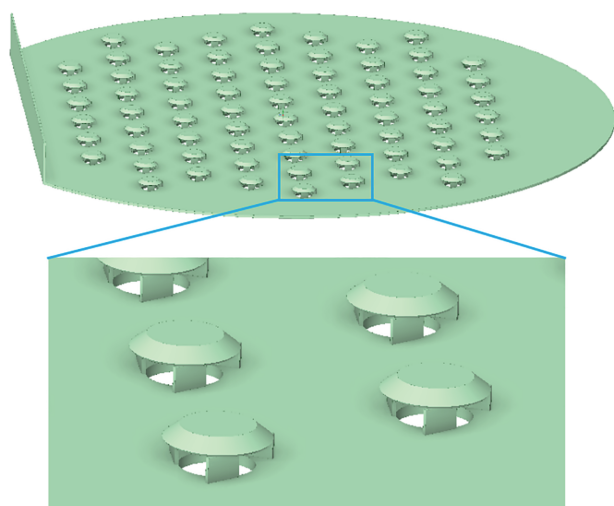


Fig. 2. The structure of the divided fixed-valve tray.

descended through the downcomer and returned to the tank. Air was introduced at the column bottom, uniformly distributed through a gas-distribution sieve tray before passing upward through the fixed-valve tray. The gas exited the column at the top after passing through a wire-gauze demister and an entrainment separator tray. Liquid and gas flow rates were measured with turbine and vortex flow meters, respectively, and controlled via valves. All experiments were performed at ambient temperature (approximately 25 °C) and atmospheric pressure under varying gas and liquid loads. The orifice kinetic energy factor (F_0) ranged from 10.2 to 25.3 Pa^{0.5}, and the overflow strength (L_W) ranged from

5.0 to 44.0 m²·h⁻¹ to cover typical industrial operating conditions. The following quantities were measured as the features and targets for subsequent model training:

2.1.1. Orifice kinetic energy factor

The orifice kinetic energy factor (F_0) characterizes the kinetic energy intensity of the gas phase through the tray orifices. It is calculated using Eq. (1):

$$F_0 = \frac{Q \times \sqrt{\rho_G}}{A} \quad (1)$$

where Q is the volumetric gas flow rate, ρ_G is the gas density, and A is the tray perforated area. This parameter generalizes gas load effects by normalizing gas density and perforation geometry, providing a more consistent indicator than volumetric flow rate.

2.1.2. Overflow strength

Overflow strength (L_W) describes the liquid loading capacity per unit weir length, as calculated in Eq. (2),

$$L_W = \frac{L}{l_w} \quad (2)$$

where L is the liquid flow volumetric rate and l_w is the overflow weir length. Larger L_W signifies a greater liquid velocity and a thicker liquid layer, thereby implying longer residence time.

2.1.3. Wet pressure drop

The wet pressure drop (ΔP) represents a key measure of tray hydraulic performance, consisting of the dry pressure drop (ΔP_G) and the hydraulic pressure drop (ΔP_L) [36,37], as defined in Eq. (3).

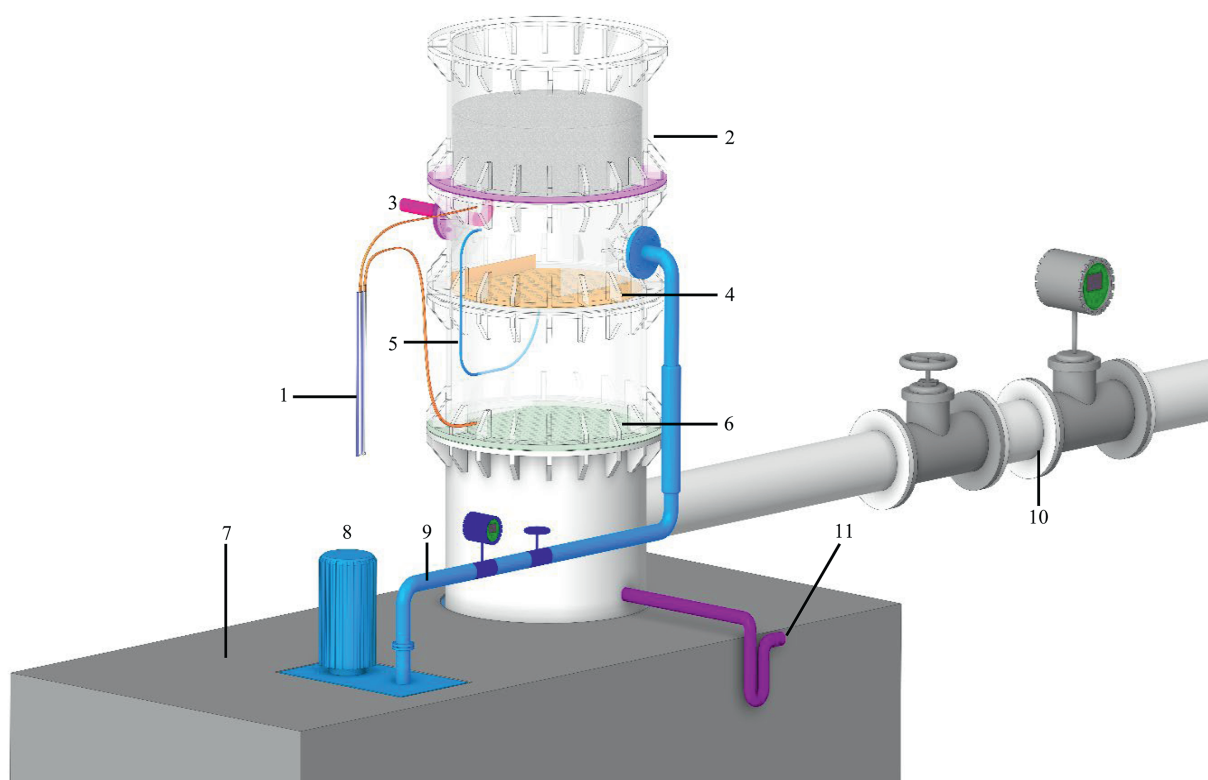


Fig. 3. The experiment device: 1, U-shaped pressure manometer; 2, Wire-gauze demister; 3, Entrainment-collection pipeline; 4, Fixed-valve tray; 5, Clear-liquid-height measurement tube; 6, Gas-distribution sieve tray; 7, Water tank; 8, Centrifugal pump; 9, Liquid-supply pipeline, valve and flowmeter; 10, Gas-supply pipeline, valve and flowmeter; 11, Weep-collection pipeline.

$$\Delta P = \Delta P_G + \Delta P_L \quad (3)$$

After reaching steady-state operation, ΔP was measured directly using a U-shaped pressure manometer. Measurements were taken across all designated operating points by adjusting the gas and liquid flow rates *via* control valves and a variable frequency drive.

2.1.4. Clear liquid height

The clear liquid height (h_{CL}) denotes the height of the liquid free from froth on the tray [38,39]. It was measured *via* a static pressure tube, following the principle in Eq. (4),

$$h_{CL} = \frac{P_{CL}}{\rho_L \times g} \quad (4)$$

where P_{CL} is the static pressure at the tray surface, ρ_L is the liquid density, and g is the gravitational acceleration. A transparent tube was connected to the tray surface and vented to the space above to eliminate demister pressure effects. The liquid column height in the tube, measured vertically from the tray surface (set as 0 m), gave the value of h_{CL} .

2.1.5. Weep rate

Weeping occurs at low gas velocities when gas momentum cannot sustain the liquid head on the tray [40]. The leaked liquid was collected through a U-bent drain line to prevent gas bypass. The weep rate (ω) was measured by weighing the mass of weeping (m_{Weep}) collected over a known time interval (Δt), calculated using Eq. (5) [41],

$$\omega = \frac{m_{Weep}}{\rho_L \times \Delta t \times L} \quad (5)$$

where L is the liquid flow volumetric rate.

2.1.6. Entrainment rate

Entrainment occurs at high gas flow rates, where liquid droplets are carried by the gas to the tray above [17,42]. The entrained liquid was collected by the demister located above the test tray. The entrainment rate (e_v) was similarly determined by gravimetric method, calculated *via* Eq. (6),

$$e_v = \frac{m_{Entrainment}}{\rho_G \times \Delta t \times Q} \quad (6)$$

where $m_{Entrainment}$ is the mass of entrained liquid collected over time Δt , and Q is the gas flow volumetric rate.

2.2. Algorithms

Based on the characteristics of the experimental data and the requirements of the prediction task, four representative ML models were initially selected from open-source Python libraries: random forest (RF), extreme gradient boosting (XGBoost), support vector regression (SVR), and a shallow multi-layer perceptron (MLP). To the best of our knowledge, this study constitutes the first comparative application of these algorithms in tray hydrodynamics prediction. Model selection considered several challenges: (a) the need to predict four continuous hydrodynamic parameters from two inputs (a multivariate regression task); (b) the small dataset size and inherent experimental noise; (c) strong nonlinearity; and (d) strong coupling between gas and liquid loads.

3. Results and Discussion

3.1. Training machine learning models and hyperparameter optimization

3.1.1. Data preprocessing

A preliminary exploratory analysis was conducted on the 760 sets of experimental data obtained from the cold-flow tray experiments. The histograms in Fig. 4 illustrate the distribution of

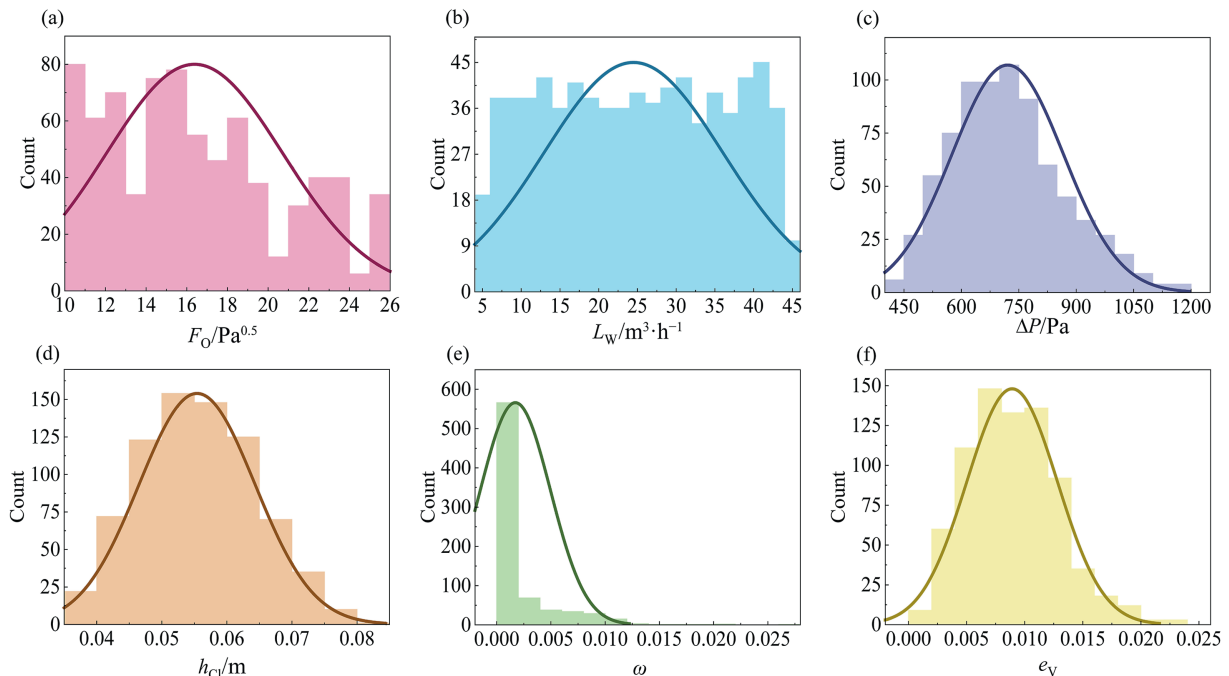


Fig. 4. Distribution of data.

the main input and output variables. The preliminary data exploration confirms that the numerical ranges and variation trends of all variables are reasonable. This indicates satisfactory overall data quality, providing a reliable foundation for subsequent modeling and analysis. As shown in Fig. 4(a), the distribution of the orifice kinetic energy factor shows a higher frequency at lower values due to intentional oversampling in that region to enhance the ML models' predictive capability for the weep rate. The histograms of weep and entrainment rates (Fig. 4(e)–(f)) show data concentration near low values, consistent with their theoretical range of [0, 1].

To eliminate unit and scale discrepancies and improve feature distribution, all variables were standardized or log-transformed before modeling. The two input features (F_0 , L_W) and two output targets (ΔP , h_{Cl}) were standardized using the StandardScaler tool from the Scikit-learn library, transforming them into standard normal distributions (mean ≈ 0 , $\sigma \approx 1$). This process enhances model convergence speed and stability. In Eq. (7), x_i represents the original data point, while $\bar{x}$ and σ denote the sample mean and standard deviation, respectively. To reduce skewness in the dimensionless outputs (ω , e_v) which are concentrated near zero, a logarithmic transformation was applied using the $\text{np. log1p}(x)$ function (Eq. (8)) from NumPy [43]. The transformed data were subsequently standardized, and inverse standardization with exponential back-transformation was performed after prediction to recover the original physical values.

$$z_i = \frac{x_i - \bar{x}}{\sigma} \quad (7)$$

$$x' = \log(x_i + 1) \quad (8)$$

3.1.2. Training and validation

To ensure methodological reliability and model robustness, several strategies were implemented before training. A dataset of 760 samples was acquired from cold-flow experiments, encompassing two input features (F_0 , L_W) and four hydrodynamic targets (ΔP , h_{Cl} , ω , e_v) for the divided fixed-valve tray under various operating conditions. After preprocessing, the dataset was randomly partitioned into training and testing subsets at a 4:1 ratio. All subsequent modeling and evaluation for the four ML algorithms were conducted using consistent partitions across all ML algorithms to avoid partition-related bias, thereby ensuring the representativeness and reliability of the model assessment. Given the relatively small sample size ($N = 760$), a 10-fold cross-validation strategy was employed to mitigate overfitting during the training phase. This approach is well-suited for limited data scenarios as it maximizes data utilization while enhancing the robustness of the evaluation [44]. Specifically, the train set was randomly divided into 10 subsets (folds). In each of the 10 iterations, nine folds were used for model training and hyperparameter optimization, while the remaining one fold was reserved for validation. Performance metrics were averaged across all folds. This procedure ensures that each data sample is used once for validation, thereby maximizing data utilization, reducing dependence on any single data split. It provides a consistent and unbiased estimate of model performance even under limited data conditions. Additionally, a dropout rate of 0.02 was applied after each hidden layer in the Shallow MLP to suppress overfitting.

All models were trained to predict the four continuous hydrodynamic targets. Based on practical engineering principles, non-negativity constraints were applied to all predictions. Performance was quantified using the Root Mean Square Error (RMSE) and the coefficient of determination (R^2) derived from the 10-fold cross-validation results. R^2 measures the proportion of variance in the target variable that is predictable from the input features, while

RMSE represents the average prediction error magnitude [45]. The corresponding calculation formulas are shown in Eqs. (9) and (10).

$$R^2 = 1 - \frac{\sum_{i=1}^n (x_i - \hat{x}_i)^2}{\sum_{i=1}^n (x_i - \bar{x})^2} \quad (9)$$

$$\text{RMSE} = \sqrt{\frac{1}{n} \sum_{i=1}^n (x_i - \hat{x}_i)^2} \quad (10)$$

3.1.3. Hyperparameter optimization

Hyperparameter optimization was performed automatically using the Optuna framework [46], which employs a Bayesian optimization approach for efficient search. In this approach, the model's validation performance (e.g., R^2 or RMSE) was defined as the objective function, and Optuna iteratively explored the parameter space to identify the optimal configuration. This procedure enhances model accuracy while reducing manual tuning effort. A log-uniform distribution was applied to parameters with large ranges to improve sampling efficiency. The search space and the optimized hyperparameters obtained for each algorithm are listed in Table 1.

3.2. Performance evaluation of ML models

The four ML algorithms (RF, XGBoost, SVR, Shallow MLP) were trained using F_0 and L_W as inputs to predict the four hydrodynamic targets. Other tray parameters remained constant. The evaluation of the ML models' predictive performance is illustrated using the RF model as an example, while results for the other three are provided in Supplementary Material A (Figs. A1–A3).

For benchmark comparison, a Model-Driven Model incorporating established theoretical correlations was constructed. The wet pressure drop was estimated by Bennett's unified model [47], the clear liquid height by Colwell [48], the weep rate by Huang *et al.* [49], and the entrainment rate by Yashin *et al.* [50]. These classical correlations served as the theoretical baseline for comparison with ML predictions. Both MDM and ML models were trained and evaluated on identical splits to ensure fair comparison. Given constant equipment and system properties, the

Table 1
Optuna hyperparameter search space and optimized results.

Model	Hyperparameter	Search Range	Optimal Value
RF	n_estimators	[100, 400]	307
	max_depth	[3, 20]	18
	min_samples_split	[2, 10]	2
	min_samples_leaf	[1, 5]	1
XGBoost	max_features	['sqrt', 'log2', None]	None
	n_estimators	[200, 500]	482
	max_depth	[3, 10]	3
	learning_rate	[0.01, 0.2]	0.195
	Subsample	[0.6, 1.0]	0.936
	colsample_bytree	[0.5, 1.0]	0.733
	reg_alpha	$[1 \times 10^{-8}, 10.0](\log)$	6.424×10^{-7}
SVR	reg_lambda	$[1 \times 10^{-8}, 10.0](\log)$	0.291
	C	$[1 \times 10^{-2}, 100.0](\log)$	73.882
	Epsilon	$[1 \times 10^{-3}, 1.0](\log)$	0.0559
	Gamma	['Scale', 'auto']	auto
Shallow MLP	hidden1	[32, 128]	66
	hidden2	[32, 128]	77
	Dropout	[0.0, 0.5]	0.0036
	learning_rate	$[1 \times 10^{-4}, 1 \times 10^{-2}](\log)$	0.0009

hydrodynamic performance primarily depends on the gas and liquid loads, allowing the theoretical calculations to be simplified functions of these two factors (Eqs. (11)–(14)).

$$\Delta P = 73.4 F_0^{0.5840} L_W^{0.2137} \quad (11)$$

$$h_{Cl} = 0.0194 + 6.22 \times 10^{-4} L_W + \frac{2.97 + 0.00307 L_W}{22.96 + 8.0464 F_0} \quad (12)$$

$$\omega = 2.12 \times 10^8 F_0^{-9.6866} L_W^{-0.3614} \quad (13)$$

$$e_v = 1.14 \times 10^{-4} F_0^{0.7640} L_W^{0.7053} \quad (14)$$

Fig. 5 shows the comparison between MDM calculations and experimental values for the train and test set. Ideally, data points should align along the 1:1 diagonal. For wet pressure drop (Fig. 5(a)), the MDM shows reasonable accuracy but underestimated values between 600 and 1000 Pa are underestimated. The clear liquid height calculations (Fig. 5(b)) show good overall agreement but with noticeable underestimation for some points between 0.062 and 0.08 m. The MDM exhibits poor performance for both the weeping and entrainment rates (Fig. 5(c)–(d)), with predictions showing wide scatter and substantial deviations from the experimental values, indicating limited predictive reliability.

In contrast, the RF model's predictions demonstrate significantly better agreement with experimental data, as shown in Fig. 6. Predictions for wet pressure drop (Fig. 6(a)) and clear liquid height (Fig. 6(b)) align closely with the diagonal, indicating high accuracy. For the weep rate (Fig. 6(c)), predictions are excellent in the low-rate region (0–0.012), where data is concentrated, with more scatter at higher, sparser rates. Entrainment rate predictions (Fig. 6(d)) are also strong in the predominant low-to-medium value range (0.002–0.015). Crucially, the RF model's performance on the test set is comparable to its performance on the training set, indicating no overfitting. The results from the other ML models (Figs. A1–A3) also consistently outperform the MDM benchmark. This demonstrates that these data-driven ML models can accurately predict the hydrodynamic performance of the divided fixed-valve tray, effectively capturing the complex nonlinear relationships inherent in the data.

3.3. Comparison and screening of ML models

The predictive performance of the proposed models was evaluated on the test set using the coefficient of determination (R^2), root mean square error (RMSE), and a comprehensive evaluation metric (R_{com}) derived from R^2 . As shown in Fig. 7(a)–(b), all ML models achieved R^2 values greater than 0.9 for the four output

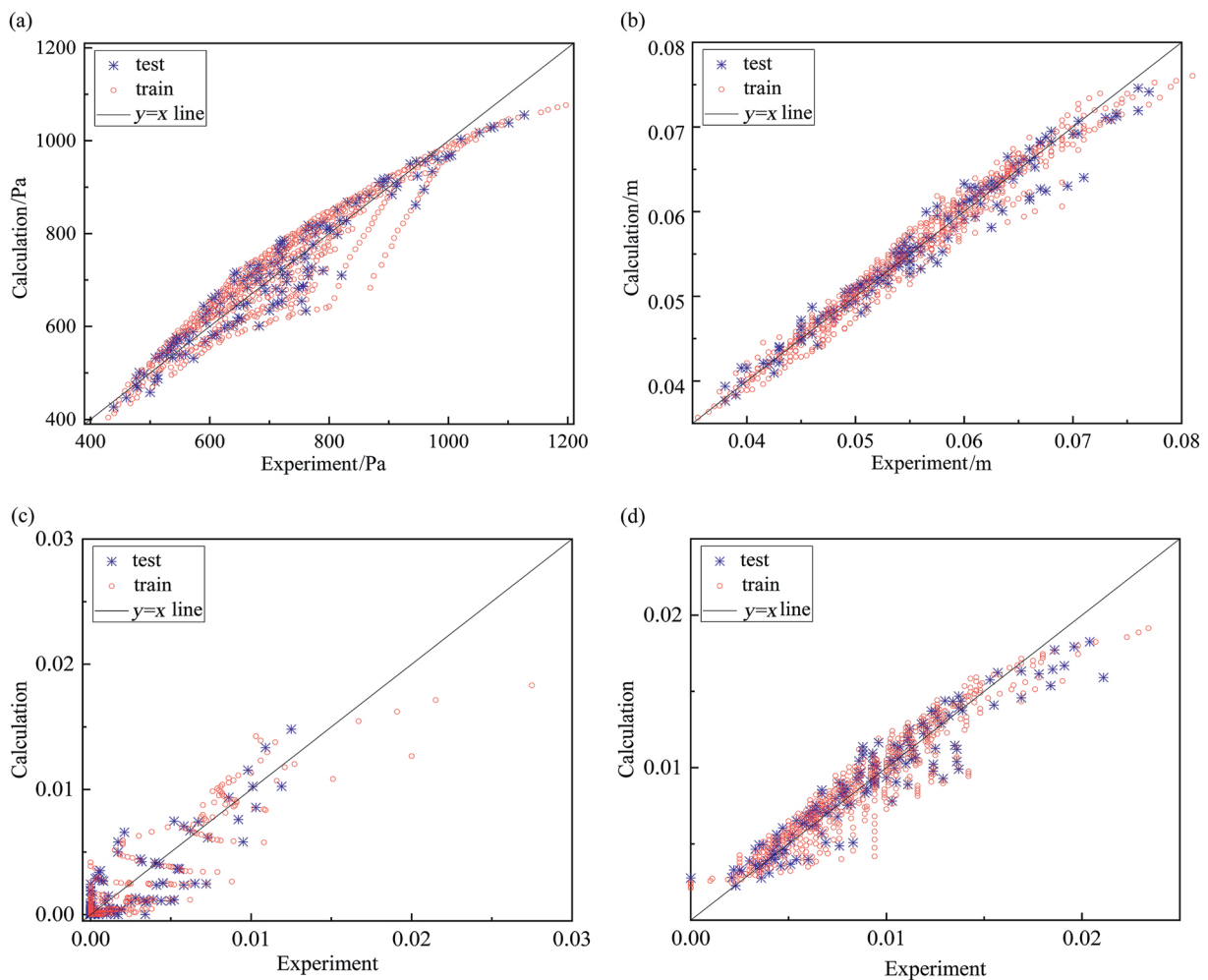


Fig. 5. Calculations vs experiments plots of MDM: (a). ΔP ; (b). h_{Cl} ; (c). ω ; (d). e_v .

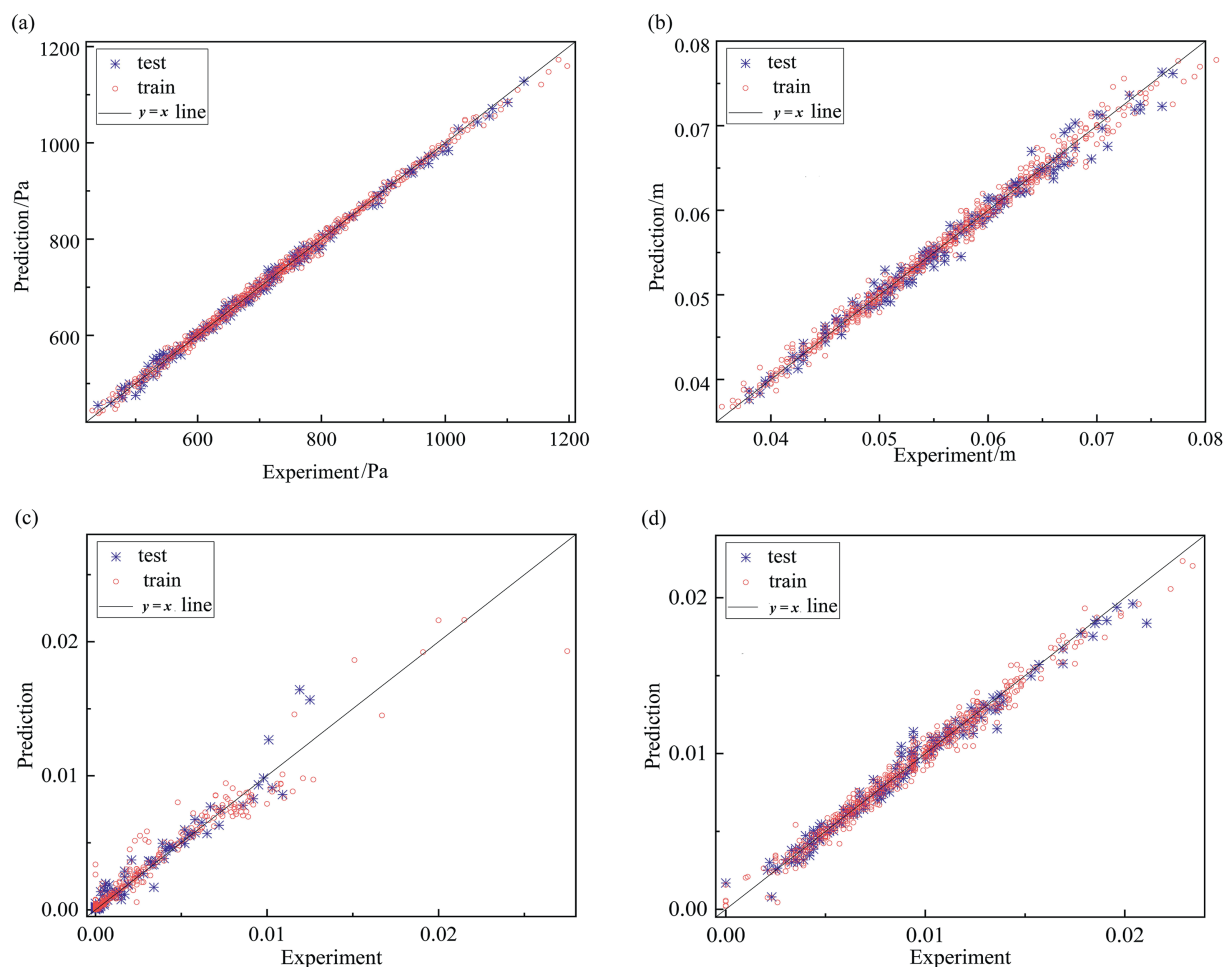


Fig. 6. Predictions vs experiments plots of RF: (a). ΔP ; (b). h_{Cl} ; (c). ω ; (d). e_v .

targets, with the exception of the Shallow MLP's slightly lower performance for the weep and entrainment rates. The ML models demonstrated exceptional accuracy in predicting the wet pressure drop, with all achieving $R^2 > 0.995$ and $RMSE < 11$ Pa, significantly outperforming the MDM. In contrast, the MDM showed its highest accuracy for clear liquid height ($R^2 = 0.9609$, $RMSE = 0.0018$ m), but performed less optimally for wet pressure drop ($R^2 = 0.9321$, $RMSE = 39.6$ Pa). An analysis of the best-performing model for each target revealed that XGBoost was superior for wet pressure drop ($R^2 = 0.9987$, $RMSE = 5.3$ Pa) and weep rate ($R^2 = 0.9871$, $RMSE = 0.0008$), Shallow MLP for clear liquid height ($R^2 = 0.9871$, $RMSE = 0.0010$ m), and Random Forest (RF) for entrainment rate ($R^2 = 0.9799$, $RMSE = 0.0006$). Overall, while the MDM showed competence for specific target, it was not the optimal model for any, indicating that the data-driven ML approaches are more effective at capturing the underlying non-linear coupled effects governing tray hydrodynamics.

Model generalization and extrapolation capabilities is a critical aspect of performance evaluation. This is essential because operational conditions encountered in real-world engineering designs are not guaranteed to fall within the range of the training data. The extrapolation capability of the models was rigorously tested on an extension set comprising 80 new data points with F_0 values of $10.0 \text{ Pa}^{0.5}$ and $26.5 \text{ Pa}^{0.5}$, which lay outside the training data range (Fig. 8). Following the same procedure as for the test set, predictions were generated for the extension set using all five models. The R^2 and RMSE were subsequently calculated for each of the four

output targets. The predictive performance of the different models on the extension set is summarized in Fig. 7(c)–(d). The MDM exhibited almost no extrapolation capability. Its best performance occurred for the clear liquid height; however, the R^2 value was only 0.0830, and the corresponding RMSE was nearly an order of magnitude higher than that obtained on the test set. XGBoost also demonstrated instability outside training range, particularly for the weep and entrainment rates, where predictions fell well outside the physically meaningful $[0, 1]$ range. In contrast, the other three ML models (RF, SVR, Shallow MLP) showed robust extrapolation performance, with most R^2 values above 0.95. The Shallow MLP performed best for ΔP and h_{Cl} ($R^2 = 0.9992$ and 0.9965 , respectively), while SVR was superior for ω and e_v ($R^2 = 0.9633$ and 0.9854). A comparison between the SVR model's extrapolated predictions and the experimental values for the extension set is presented in Fig. 9. (see Supplementary Material Figs. B1–B4 for the remaining models). Notably, the SVR model on the extension set even outperformed its test-set results, exhibiting higher R^2 and lower RMSE values overall. This enhancement indicates that the SVR model successfully learned the underlying hydrodynamic relationships rather than memorizing data. This strong generalization suggests that the SVR-based DDM possesses high predictive reliability and practical applicability.

Given that different ML models performed best for different targets or stages, and that the hydrodynamic parameters vary in engineering importance, a comprehensive evaluation metric

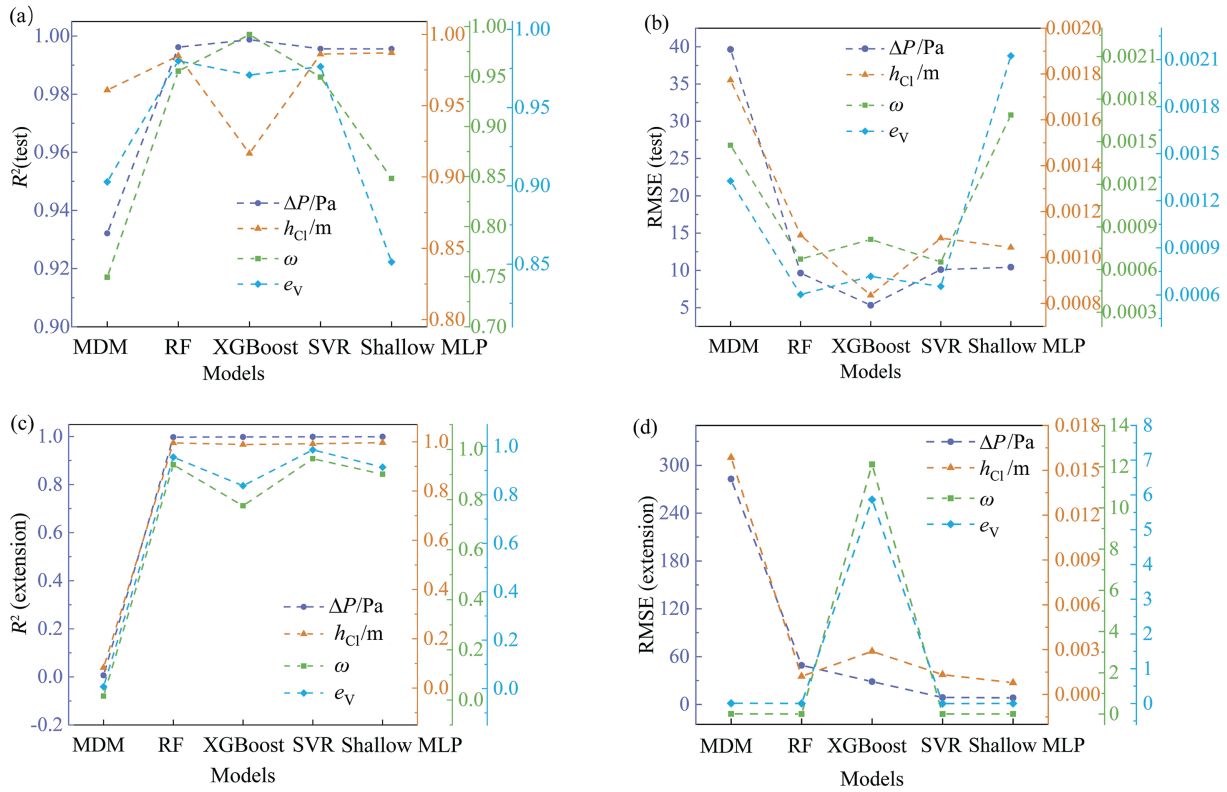


Fig. 7. Performance of models.

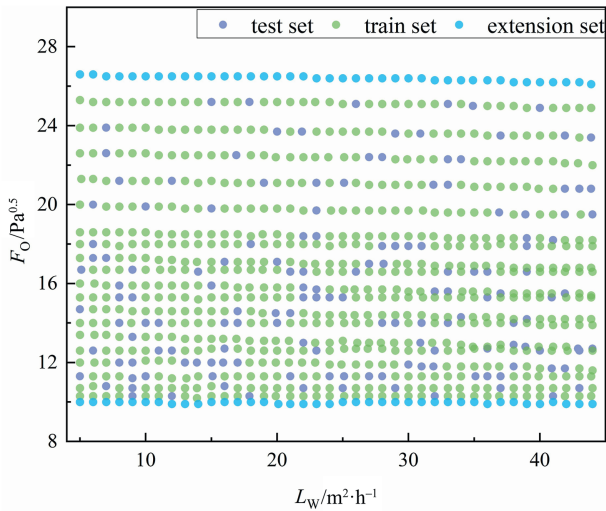


Fig. 8. Distribution of feature ranges across datasets.

(R_{com}) was introduced for a unified comparison. This metric integrates the models' R^2 values from both the test set ($R_{\text{com,t}}$) and the extension set ($R_{\text{com,e}}$), weighted by the relative importance (w_i) of each target (i): ΔP ($w_1 = 0.3$), h_{Cl} ($w_2 = 0.1$), ω ($w_3 = 0.3$), and e_v ($w_4 = 0.3$). These weights reflect the relative engineering significance of parameters. Higher weights were assigned to ΔP , ω and e_v , whereas a lower weight was assigned to h_{Cl} . This weighting reflects their relative engineering significance: ΔP directly influences energy consumption, while ω and e_v critically affect mass-transfer efficiency, whereas h_{Cl} plays a comparatively minor role. The final R_{com} is calculated as follows:

$$R_{\text{com,t}} = \sum_{i=1}^4 R_{i,t}^2 \times w_i \quad (15)$$

$$R_{\text{com,e}} = \sum_{i=1}^4 R_{i,e}^2 \times w_i \quad (16)$$

$$R_{\text{com}} = \frac{R_{\text{com,t}} + R_{\text{com,e}}}{2} \quad (17)$$

As summarized in Fig. 10, $R_{\text{com,t}}$ values for RF, XGBoost, and SVR were similar and high (0.9750–0.9801), while values for the Shallow MLP and MDM were lower. For extrapolation ($R_{\text{com,e}}$), SVR and Shallow MLP scores increased, while others decreased, with the MDM scoring lowest (0.0171). Consequently, SVR achieved the highest overall R_{com} (0.9792), identifying it as the most suitable model for this prediction task. It accurately captures the complex nonlinear relationships, demonstrates scientific reliability, and possesses superior generalization capability, performing excellently even under extrapolation conditions. In conclusion, ML models, particularly SVR, serve as reliable data-driven surrogates with strong potential for predicting the hydrodynamic performance of the divided fixed-valve tray.

3.4. Feature study

A key advantage of ML is its capacity to incorporate a broad set of input features at the start of model training, thereby ensuring the inclusion of potentially relevant physical descriptors. In this study, we expanded the original feature set comprising the orifice kinetic energy factor (F_0) and the overflow strength (L_W) by engineering five new features: F_0^2 , L_W^2 , $F_0 L_W$, F_0/L_W and L_W/F_0 . This

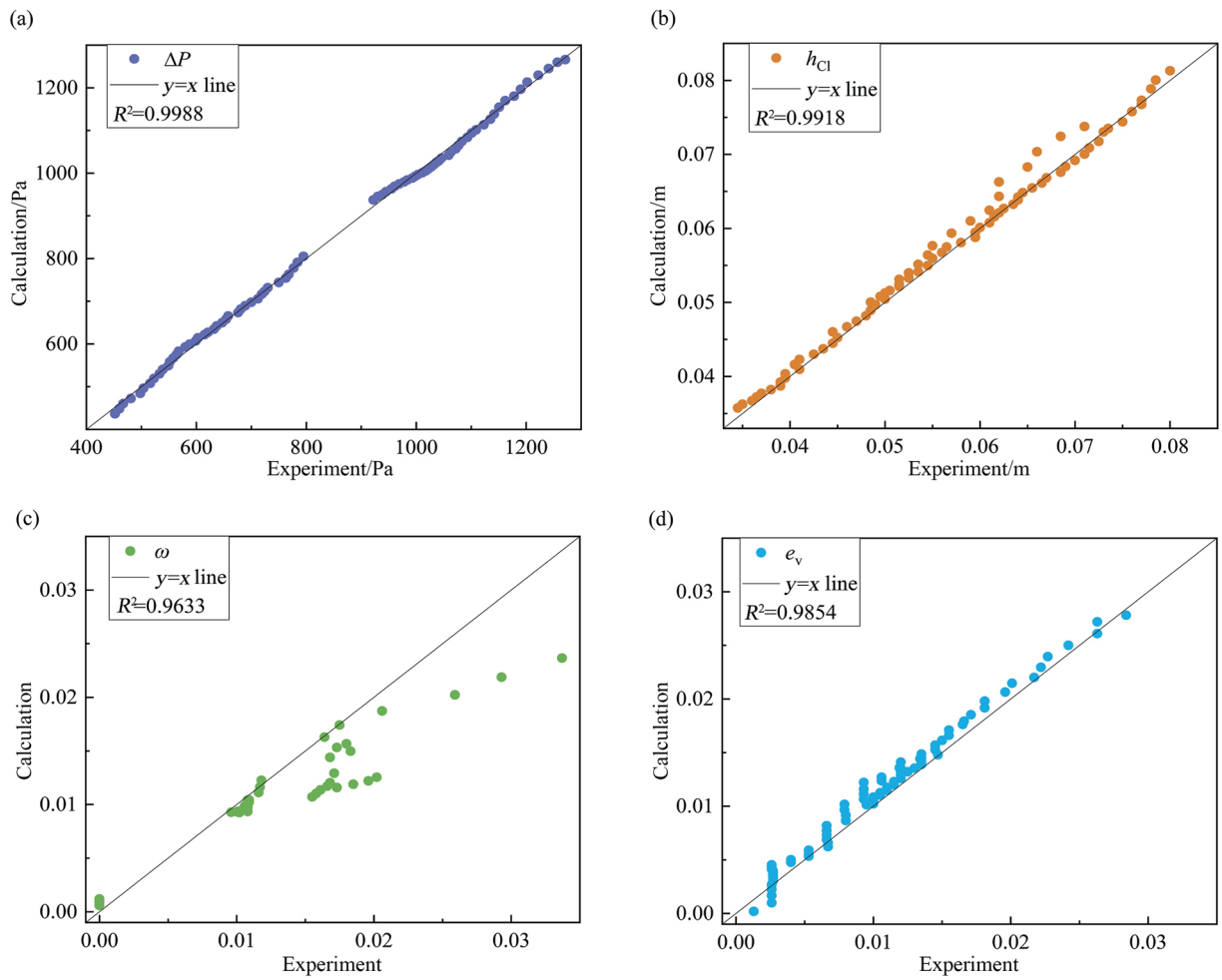


Fig. 9. Extensions vs experiments plots of SVR.

comprehensive set was utilized for subsequent feature selection and analysis based on the SVR model.

Fig. 11 illustrates the correlation matrix of the initial and engineered features. Blue and red color tones denote negative and

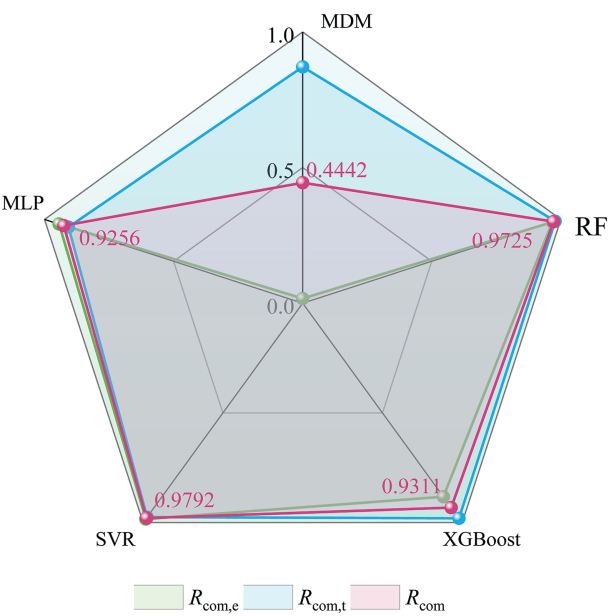


Fig. 10. Comprehensive evaluation metrics of models.

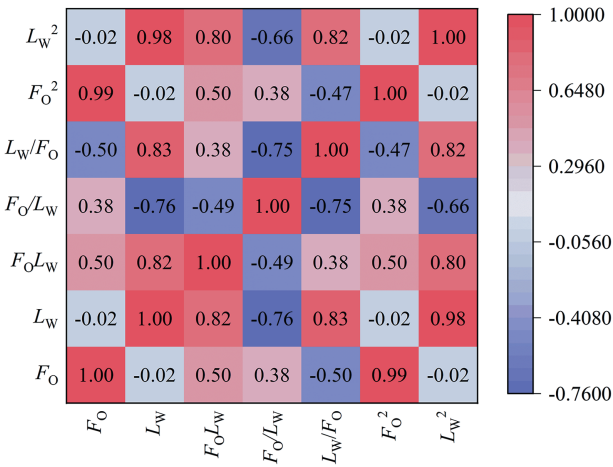


Fig. 11. Pearson correlation matrix between features.

positive correlations, respectively, with color intensity indicating the strength of the relationship. As expected, L_W exhibits strong correlation with L_W^2 , as well as F_O with F_O^2 . Although several parameters show substantial cross-correlations, all features were temporarily retained at this stage because each transformation carries distinct physical significance. Identifying the most informative features can also guide future data-collection strategies for related applications.

Analyzing feature importance is crucial for both developing and interpreting ML models. It identifies which inputs significantly influence the predictions and thus enhances transparency and reliability [51]. Such insight allows for informed feature selection, enabling removal of redundant variables and potential simplification of the model. In this work, feature importance was quantified using SHAP (Shapley Additive Explanations), a game-theoretic method that provides a consistent measure of each input's marginal contribution relative to a reference prediction [52].

The overall importance of each feature for predicting the four hydrodynamic parameters is summarized in Fig. 12, which plots the mean absolute SHAP value for each feature across the dataset. A larger mean absolute SHAP value indicates a greater influence on the model's predictions. For the wet pressure drop, F_O , F_O^2 and $F_O L_W$ emerged as the dominant predictors. For the clear liquid height, the ratio L_W/F_O plays the dominant role. The weep rate is primarily influenced by L_W/F_O , F_O , and L_W . For the entrainment rate, the engineered features L_W^2 and $F_O L_W$ exhibit higher importance than the base features L_W and F_O . Notably, the interaction term $F_O L_W$ significantly influences both ΔP and e_v , while the ratio L_W/F_O strongly governs both h_{CL} and ω .

Beyond ranking importance, it is essential to examine whether each feature contributes positively or negatively to predictions. Fig. 13 displays the SHAP summary plots, where each point corresponds to a sample and color denotes the feature magnitude (red for high, blue for low). Positive SHAP values indicate an increase in the predicted target relative to the baseline, while negative values indicate a decrease. A wider horizontal spread indicates a broader range of influence. Feature-dependence plots for all four targets are provided in the Supplementary Material (Figs. C1–C4).

As shown in Fig. 13(a), F_O , F_O^2 and $F_O L_W$ consistently exhibit positive SHAP values, indicating that increasing these features raises ΔP . Increasing any of these features results in higher wet pressure drop. The wider spread of points at lower F_O values suggests a more pronounced effect on reducing ΔP in that regime, whereas $F_O L_W$ exerts a stronger effect at higher values. Consistent with Fig. C1, F_O and L_W both show approximately linear positive effects, while $F_O L_W$ displays a strong linear dependence, confirming that ΔP is predominantly governed by F_O and its nonlinear transformations. L_W contributes only weakly, and ratio-type features are negligible. Therefore, F_O serves as the primary operational lever for adjusting ΔP in industrial applications.

For clear liquid height (Fig. 13(b)), L_W/F_O is the dominant predictor. Larger L_W/F_O corresponds to higher SHAP values and therefore higher h_{CL} . The inverse ratio F_O/L_W has the opposite but weaker influence. Thus, h_{CL} is predominantly controlled by the ratio feature L_W/F_O . Monitoring L_W/F_O in practice can help avoid unstable operating regions.

According to Fig. 13(c), the ratio L_W/F_O is the most influential feature for ω . Both low and high values of this ratio have a wide distribution of SHAP values, indicating that decreasing it can

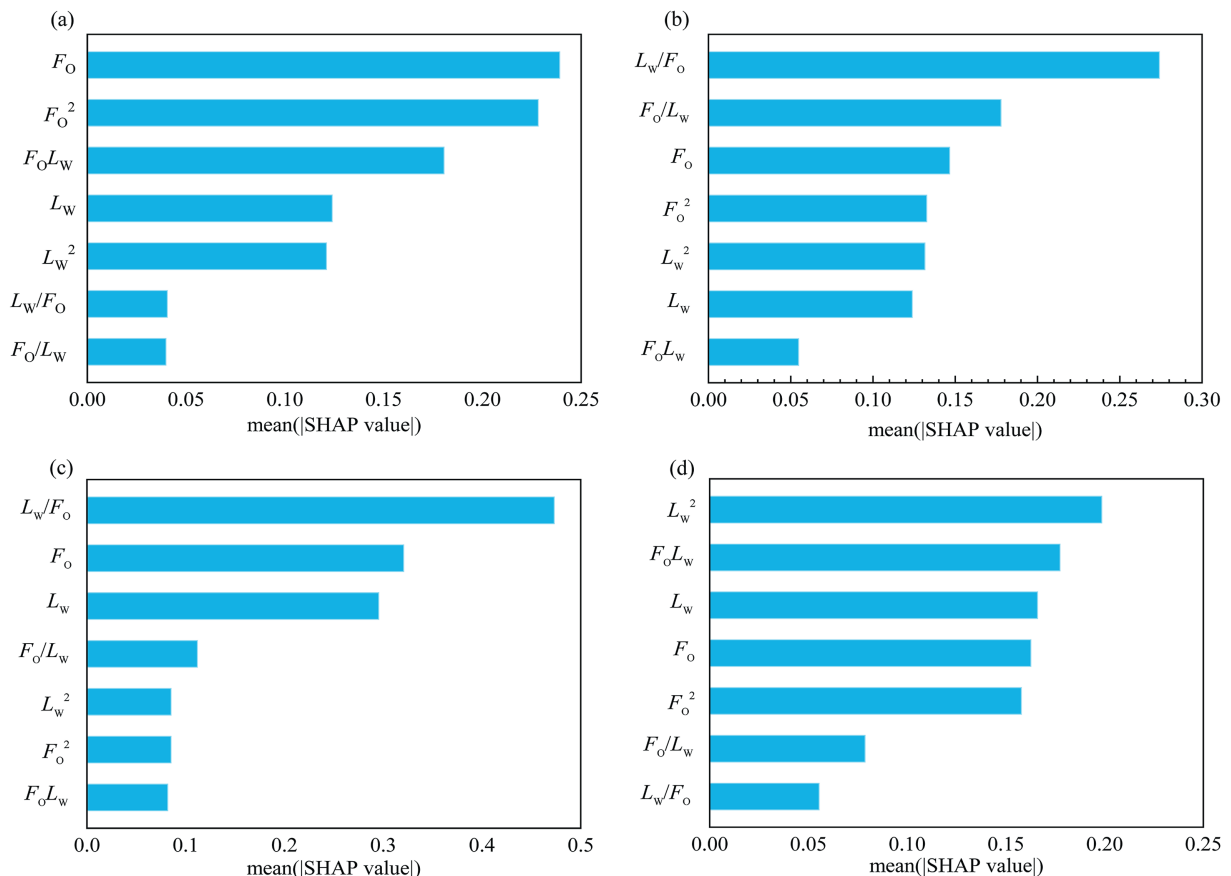


Fig. 12. Global feature importance plots: (a). ΔP ; (b). h_{CL} ; (c). ω ; (d). e_v .

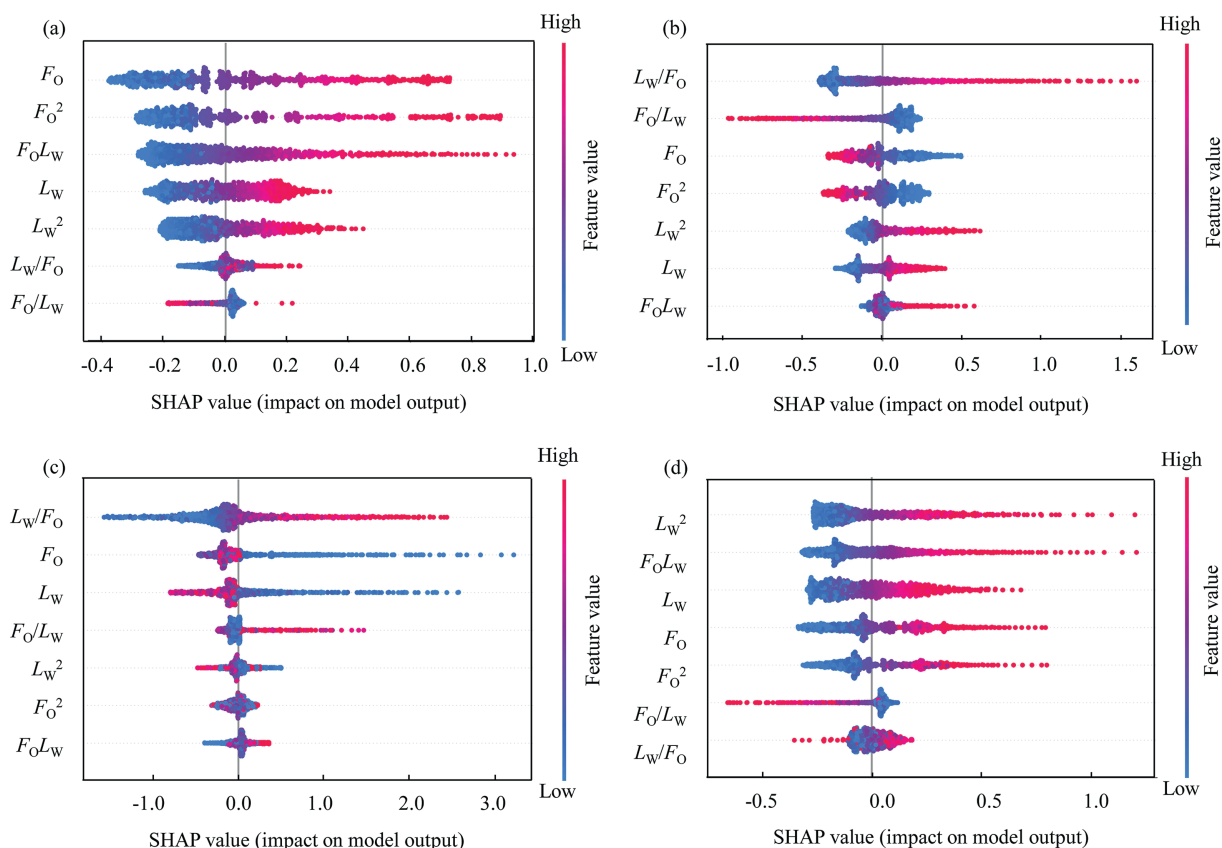


Fig. 13. SHAP summary plots: (a) ΔP ; (b) h_{CL} ; (c) ω ; (d) e_v .

significantly reduce ω , while increasing it enhances the weeping. High L_W values are associated with negative SHAP contributions—a seemingly counterintuitive result. This behavior arises from the strong correlation between L_W and L_W/F_O (Pearson coefficient = 0.83), as shown in Fig. 11. The primary positive effect is absorbed by L_W/F_O , while L_W is assigned a negative weight to maintain model balance. As shown in Supplementary Material Fig. D1, after removing only L_W/F_O , the high values of L_W are more concentrated on the right side, and their distribution is broader compared to the left side. This result further confirms the validity of the aforementioned inference. Therefore, This indicates that retaining L_W/F_O while excluding L_W may improve model robustness by reducing multicollinearity.

Fig. 13(d) shows that L_W^2 and $F_O L_W$ show strong positive contributions, with SHAP values increasing as these features increase. Lower $F_O L_W$ corresponds to negative SHAP values. And their wider distribution compared with L_W^2 indicates that adjusting $F_O L_W$ is more effective for controlling entrainment. When both F_O and L_W are low, decreasing F_O provides a stronger suppressive effect. The strictly linear relationship between $F_O L_W$ and its SHAP value (Fig. C4 in Supplementary Material C) identifies it as a key linear driver. Overall, e_v is dominated by strong nonlinear features L_W^2 , with the interaction term $F_O L_W$ representing a critical interaction mechanism.

In summary, This study demonstrates that an SVR-based data-driven framework can effectively disentangle the positive and negative influences of F_O and L_W on the four hydrodynamic indicators. By explicitly constructing and analyzing interaction features, the present work provides new insights into tray hydrodynamics and offers a valuable perspective for performance evaluation and operational optimization.

4. Conclusions

This study systematically evaluated the performance of four ML models in predicting the hydrodynamic performance of a divided fixed-valve tray and subsequently developed a hybrid framework integrating a data-driven modeling (DDM) with Interpretable machine learning. The results demonstrate that the ML-assisted data-driven approach holds a significant advantage over traditional model-driven methods for predicting wet pressure drop, clear liquid height, weep rate, and entrainment rate. Its superiority is particularly evident in capturing complex and nonlinear couplings among the variables.

Among the models compared, support vector regression (SVR) exhibited the best overall predictive performance and generalization ability, achieving the highest comprehensive evaluation score ($R_{com} = 0.9792$, comprising $R_{com,t} = 0.9750$ for the test set and $R_{com,e} = 0.9834$ for the extension set). Notably, the SVR model maintained stable and high accuracy even under extrapolated conditions beyond the training domain, demonstrating its robustness and its ability to capture the underlying physical principles governing tray hydrodynamics.

Building upon this foundation, the engineered feature analysis further clarified the governing factors behind tray hydrodynamics and highlighted the value of incorporating physically meaningful transformations. SHAP-based interpretation revealed consistent patterns across all four targets, offering transparent evidence of how kinetic and hydraulic interactions shape tray performance. These insights complement the optimization framework by identifying the most influential operational levers, thereby improving both model interpretability and practical relevance. Overall, the integrated approach provides a reliable decision-support tool for

evaluating tray behavior and guiding the design and operation of high-efficiency contacting equipment.

CRedit Authorship Contribution Statement

Peng Wang: Writing – review & editing, Writing – original draft, Methodology, Investigation, Data curation. Xing Yuan: Visualization, Software, Formal analysis. Kehan Wang: Software, Investigation, Funding acquisition. Shiji Xu: Software, Formal analysis, Conceptualization. Jiaxing Xue: Supervision, Project administration, Conceptualization. Huan Wang: Resources, Investigation. Xiuhua Wu: Methodology, Data curation. Hongkang Zhao: Writing – review & editing, Supervision, Project administration. Qunsheng Li: Writing – review & editing, Supervision, Project administration, Funding acquisition.

Declaration of Generative AI and AI-assisted Technologies in the Writing Process

Statement: During the preparation of this work, the authors used ChatGPT by OpenAI in order to assist with language polishing and manuscript refinement. After using this tool, the authors reviewed and edited the content as needed and take full responsibility for the content of the published article.

Declaration of Competing Interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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Supplementary Material

Supplementary data to this article can be found online at <https://doi.org/10.1016/j.cjche.2026.01.019>.

Nomenclature

A	perforated area of tray, m^2
e_v	entrainment rate
F_O	orifice kinetic energy factor, $\text{Pa}^{0.5}$
g	acceleration of gravity, $\text{m} \cdot \text{s}^{-2}$
h_{Cl}	clear liquid height, m
L	liquid phase volumetric flow rate, $\text{m}^3 \cdot \text{h}^{-1}$
L_W	overflow strength, $\text{m}^2 \cdot \text{h}^{-1}$
l_W	overflow weir length, m
m_{Weep}	weep amount, kg
$m_{\text{Entrainment}}$	entrainment amount, kg
n	number of data points
P_{Cl}	static pressure at the tray surface, Pa
ΔP	wet pressure drop, Pa
ΔP_G	dry pressure drop, Pa
ΔP_L	hydraulic pressure drop, Pa
Q	gas phase volumetric flow rate, $\text{m}^3 \cdot \text{h}^{-1}$
R^2	coefficient of determination
RMSE	root mean square error
R_{com}	comprehensive evaluation metric
$R_{\text{com,e}}$	comprehensive evaluation metric for extension set
$R_{\text{com,t}}$	comprehensive evaluation metric for test set

$R_{\text{t,e}}^2$	coefficient of determination of each target in the extension set
$R_{\text{t,t}}^2$	coefficient of determination of each target in the test set
Δt	collection time, s
w_i	weight value of each target in comprehensive evaluation metrics
x_i	experimental value
$\hat{x}_i$	predicted value
$\bar{x}$	mean of experimental value
x'	logarithmic target value
z_i	standardized target value
ρ_G	gas density, $\text{kg} \cdot \text{m}^{-3}$
ρ_L	liquid phase density, $\text{kg} \cdot \text{m}^{-3}$
ω	weep rate

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