EXPLAINABLE MACHINE LEARNING-BASED PREDICTION OF MIXING EFFICIENCY IN PASSIVE MICROFLUIDIC MICROMIXERS USING EXPERIMENTAL DATA

Kingsley Obinna Iwuji *Department of Mechanics and Machine Design, Faculty of Mechanical Engineering, Opole University of Technology, Opole, Poland.* *(+ Corresponding author)*
Email: koiwuji1989@gmail.com

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ABSTRACT

In microfluidic systems, passive micromixers play crucial roles by ensuring fluid is well-mixed in microscale channels without the need for external energy input. However, there is a significant challenge in the design of passive microfluidic devices to obtain efficient mixing under laminar flow. An explainable machine learning framework was designed to predict mixing efficiency in passive microfluidic micromixers, using experimentally obtained data. The experimental data from the zigzag and split-flow micromixer configuration was used to assess the effect of flow rate, Reynolds number, viscosity and design on mixing performance. Three regression-based machine learning models, namely Linear Regression, Decision Tree Regressor and Random Forest Regressor, were developed and tested with Root Mean Square Error (RMSE) and coefficient of determination (R^2) metrics. The model with the best predictive performance was the Linear Regression model which had a value of RMSE equal to 0.0207 and R^2 equal to 0.8827, showing good agreement between the mixing index values predicted and experimental. Explainable artificial intelligence analysis using SHAP and feature-importance evaluation revealed that flow rate and Reynolds number were the dominant factors influencing mixing efficiency, while viscosity exhibited a negative effect on mixing performance. The results show the viability of combining microfluidic data from experiments with explainable machine learning methods to analyze and optimize passive micromixers. The proposed framework offers a meaningful and efficient solution to the problem of repeated experiments and CFD-based optimization in microfluidic system design.

Contribution/Originality: This study contributes to the existing literature by integrating experimentally obtained passive micromixer data with explainable machine learning for mixing-efficiency prediction. It is one of the few studies to combine predictive modelling with SHAP-based interpretability, demonstrating that flow rate and Reynolds number are the dominant factors influencing mixing performance.

1. INTRODUCTION

Microfluidics has emerged as an important technological field for manipulating small volumes of fluids within microscale channels and has found extensive applications in biomedical diagnostics, chemical synthesis, drug delivery, and lab-on-chip systems [1]. In these systems, micromixers play a vital role in facilitating the mixing of several fluids to ensure homogeneous concentration distributions that are required for efficient chemical and biological processes [1]. The simplicity, low fabrication cost and the integration into compact microfluidic devices has made passive micromixers a subject of much interest [1]. However, fluids flowing in microchannels are mostly laminar because the Reynolds numbers involved in microscale systems are small. Laminar flow regimes are characterized by fluids flowing in parallel layers with little turbulence, and thus little interaction across the interfaces, and little molecular diffusion between the fluid layers [1]. Therefore, one of the most important issues for passive microfluidic devices is the rapid and efficient mixing.

To overcome this limitation, a myriad of passive micromixer geometries have been suggested to improve the mixing performance by enhancing the chaotic advection and the interfacial stretching, including zigzag channels, split and recombine structures, serpentine channels and obstacle-based channels [1]. In the last few years, computational fluid dynamics (CFD), optimization algorithms and machine-learning methods have become more prevalent in microfluidic research to help speed up the design of microfluidic mixers and predict their performance

[2]. Previous work has shown that machine learning models can be trained on CFD-generated and experimental data to accurately predict mixing efficiency, pressure drop, and flow characteristics [3, 4]. Various optimization approaches that employ machine learning, surrogate modelling and metaheuristic algorithms have also been developed to identify optimized micromixer geometry and operating conditions [3, 4]. Moreover, AI has demonstrated significant promise in minimizing computational expenses due to redundant and repetitive CFD simulations and in optimizing the design exploration process in microfluidic systems [2].

While significant progress has been made, there are still critical drawbacks in the current research on AI-enhanced micromixers. Previous studies are mostly focused on the prediction accuracy and optimization performance and neglect the model interpretability and explainability [3, 4]. This has forced many to develop machine learning models where the mixing behaviour is predicted by a black-box system, where it is hard to define or determine the contributions of individual geometric and operational parameters to the predicted mixing behaviour. In the field of scientific and engineering applications, explainable artificial intelligence (XAI) and interpretable surrogate modelling have recently been brought to the fore with their aim of providing transparency and interpretability in machine learning systems [5]. But, the applicability of explainable machine learning techniques to passive microfluidic micromixer research is still relatively under-explored, especially when using experimental data sets instead of solely data sets generated in a computational environment. This opens the possibility of a void in the evolution of explainable AI frameworks that not only can predict mixing efficiency, but could also give engineering insight into how flow rate, viscosity, and geometry influence micromixer performance.

Therefore, this study aims to develop an explainable machine learning model for predicting mixing efficiency in passive microfluidic micromixers using experimental data. In particular, the study employs the digitized experimental data from passive micromixer geometries and uses regression-based machine learning (ML) techniques as well as explainable artificial intelligence (XAI) analysis to assess the effects of operational and geometric parameters on mixing performance. The study contributes to existing literature by integrating experimental micromixer data with interpretable machine learning methods capable of providing both predictive capability and engineering transparency.

The rest of this paper is organized as follows: In Section 2, the materials and methods are introduced, such as dataset preparation, preprocessing, machine learning models, evaluation metrics, and explainable AI techniques. The results from the experiments, machine learning, explainability analysis, and discussion of the findings are presented in Section 3. Finally, Section 4 summarizes the main conclusions and gives some suggestions for future studies.

2. MATERIALS AND METHODS

2.1. Experimental Dataset

The data set employed in this work was taken from the experimental study on the passive micromixer that was previously reported by Iwuji and Gadanya [1]. The original study compared and evaluated experimentally the mixing performance of three passive micromixer geometries, namely straight-channel, zigzag-channel and flow-splitting-channel configurations, with varying flow conditions. In the experimental setup, microfluidic devices were fabricated utilizing 3D printing technologies, and characterization of fluid mixing was carried out by optical visualization and grayscale intensity analysis [1]. Data for the experimental work done for the present study were obtained from the zigzag and flow-splitting geometries as these two geometries were seen to achieve significant mixing improvement over the straight-channel geometry [1]. The chosen data set comprised the measured values of mixing-indices obtained by experiments under different flow rates. The machine learning set was also expanded to include additional mixing data from the flow-splitting geometry that is viscosity dependent. The most important variables obtained for analysis were flow rate (mL/min), dynamic viscosity (mPa.s), geometry type and mixing index. The mixing index was used as the output variable to assess the level of homogeneity of the fluid within the micromixer channel. Flow rate and viscosity were considered as continuous numerical variables, and the micromixer geometry was considered as a categorical design variable. The final dataset was created by combining experimentally reported mixing-index and flow characterization observations from the previous study of Iwuji and Gadanya [1]. Numerical

observations were systematically extracted, organised and structured into a dataset suitable for machine learning based prediction modelling and explainable artificial intelligence analysis.

2.2. Data Preprocessing

The experimental data was preprocessed to make it compatible with the machine learning model and enhance the predictive capability before the machine learning analysis. The first step was to clean and organize the data in a consistent manner, such as flow-rate, viscosity, and mixing-index observations. The selected experimental observations were directly taken from the reported figures and summarized performance results [1] and hence no missing values were observed within the extracted dataset. The categorical geometry variable has been transformed to a numerical one to facilitate machine learning processing. The zigzag geometry was given a score of 0 and the flow-splitting geometry a score of 1. Previous studies on micromixers using machine learning had similar preprocessing methods that included encoding of the design variables and structured preparation of the datasets [6]. Scale differences among the numerical variables were then minimized by performing feature normalization and stabilizing the regression model. This was followed by splitting the dataset into training and testing sets, to evaluate the developed models predictively. The training dataset was used for model learning, while the testing dataset was used to assess predictive generalization and model accuracy.

2.3. Machine Learning Models

In this work, three regression models based on machine learning were used to predict the mixing efficiency for the experimental data set of the micromixer. These models were chosen due to their ability to be used for small structured data sets, as well as their performance in regression-based engineering prediction tasks.

2.3.1. Linear Regression

In order to set up the linear relationship between the input variables and mixing index, Linear Regression was implemented as a baseline predictive model. The model calculates the target output as a weighted linear sum of the predictor variables: geometry type, flow rate and dynamic viscosity.

2.3.2. Decision Tree Regressor

The Decision Tree Regressor was used to test the nonlinear relationships in the experimental data. The model is recursive partitioning, where the feature space is divided into decision regions defined by thresholds of the predictor variables. These methods allow capturing the complex interplay involving geometry, viscosity and flow conditions impacting mixing.

2.3.3. Random Forest Regressor

Random Forest Regressor was used as an ensemble-learning model which is based on multiple decision trees built on random sub-sets of the data. Ensemble averaging mechanism provides a more stable prediction than individual decision trees, and reduces overfitting. Random Forest models are especially well suited to engineering data with small sample sizes and nonlinear interaction between the parameters.

2.4. Model Evaluation Metrics

For the predictive performance of the machine learning models, Root Mean Square Error (RMSE) and the coefficient of determination (R^2 score) were used. The RMSE quantity was used to measure the "size" of prediction errors of the actual and predicted mixing-index values, and the R^2 score was used to measure how much variance in the mixing-index data was explained by the predictive model.

RMSE

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

R^2 Score

$$R^2 = 1 - \frac{\sum (y_i - \hat{y}_i)^2}{\sum (y_i - \bar{y})^2} \quad (2)$$

Lower RMSE values indicate improved predictive accuracy, whereas higher R^2 values indicate stronger agreement between predicted and experimental mixing-index observations.

2.5. Explainable AI Analysis

Explainable artificial intelligence (XAI) analysis was applied to improve the interpretability and engineering transparency, in this case by applying SHAP (SHapley Additive exPlanations). SHAP analysis offers quantitative information on the impact that a single input variable has on the model's prediction, and can also be used to identify variables with the greatest impact on the mixing efficiency [7].

The relative importance of the three variables, flow rate, geometry type, and dynamic viscosity in the prediction of the mixing index was performed using a feature-importance analysis method. In the field of fluid-processing systems, explainable machine learning methods have been shown to be effective in understanding and learning the micromixing behaviour, as well as in detecting and understanding key operational parameters [5, 7]. In this study, SHAP analysis was used to provide interpretable insights into the relationship between the variables of the micromixer design and the predictions of mixing performance.

3. RESULTS AND DISCUSSION

3.1. Experimental Mixing Characteristics

3.1.1. Effect of Geometry

The experimental data showed that the geometry of the micromixer played a key role in the mixing efficiency. The mixing-index values for the split-flow micromixer were always higher than those for the zigzag geometry, as indicated in Figure 1, throughout the range of flowrates considered. The mixing-index values between approximately 0.66 and 0.96 were obtained for the split-flow configuration, while the zigzag geometry's mixing-index values were between approximately 0.68 and 0.95. This superior performance of the split-flow geometry is due to the repeated fluid splitting and recombination mechanisms which increase the stretching and chaotic advection at the interfaces inside the microchannel [1]. The mixing efficiency also improved progressively with flow rate for the zigzag geometry, suggesting that the curvature of the channels and the channel-direction changes facilitated fluid-interface deformation and improved the mixing efficiency. The split-flow geometry did, however, exhibit greater mixing augmentation mechanisms at relatively lower flow rates indicating quicker mixing augmentation enhancement [5, 7]. The same effect of geometric modification to significantly enhance fluid mixing behaviour and reduce mixing length requirements has been observed in previous CFD-assisted and machine-learning-assisted micromixer studies [3, 4]. The results accordingly support that the micromixer geometry is an essential parameter that affects the passive microfluidic mixing performance. Results indicated that while the operational parameters had significant influence on mixing efficiency, the geometric changes increased the interaction between the fluids and thus the effectiveness of mixing.

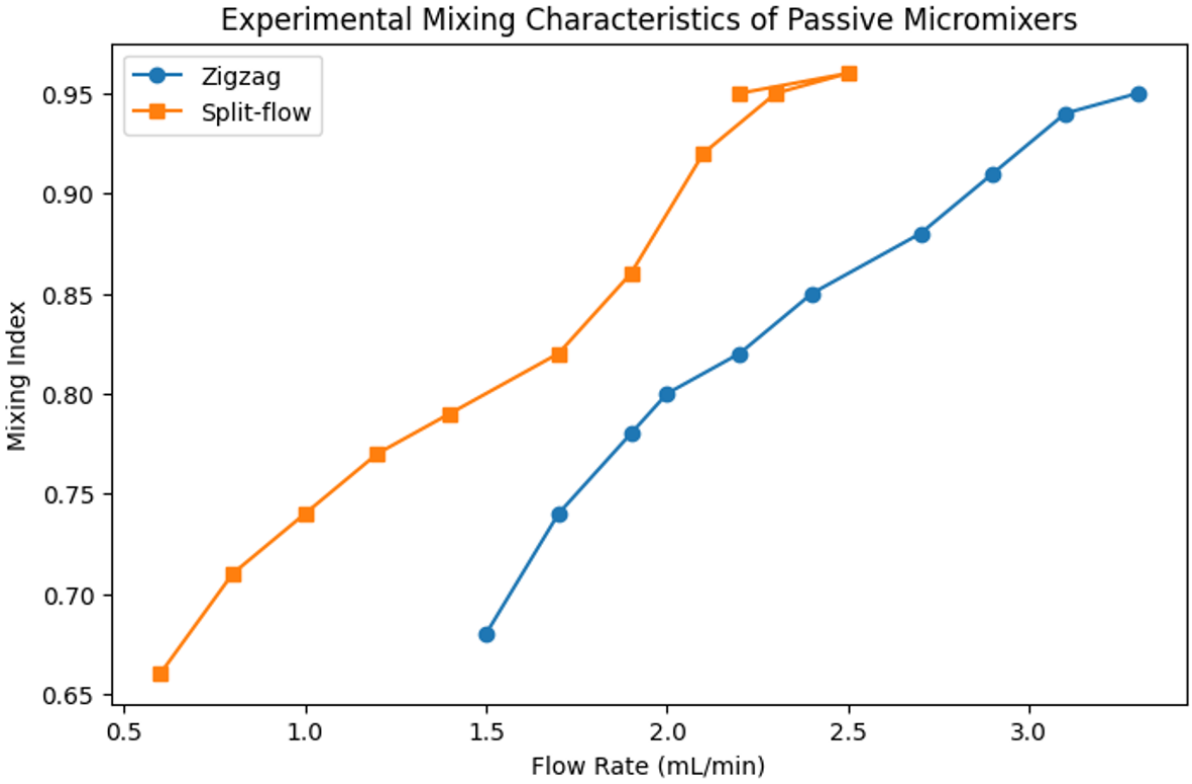

Figure 1. Experimental mixing characteristics of zigzag and split-flow passive micromixers under varying flow conditions.

3.1.2. Effect of Flow Rate

Overall, the experimental results showed an improvement in mixing efficiency with higher flow rate for both micromixer designs as seen in Figure 2. The mixing index also increased for the zigzag micromixer from ~0.68 at 1.5 mL/min to ~0.95 at 3.3 mL/min, and for the split-flow geometry from ~0.66 at 0.6 mL/min to ~0.96 at 2.5 mL/min. The improved mixing efficiency with flow rates observed here is due to enhanced convective transport and greater stretching of the interface at higher Reynolds numbers. The higher the flow rates are, the more the fluid is deforming and the greater the mixing area between fluid streams, leading to better mixing in the microchannel. Passive micromixing enhancement caused by Reynolds number also has been reported previously in CFD and optimization studies of passive microfluidic systems [8, 9]. The flow rate/mixing efficiency correlation obtained in the present work suggests that the operational flow conditions play a significant role in the passive micromixer's performance. The results also indicate that the enhancement in chaotic advection and convective mixing in passive microfluidic devices is in favor of a higher Reynolds number.

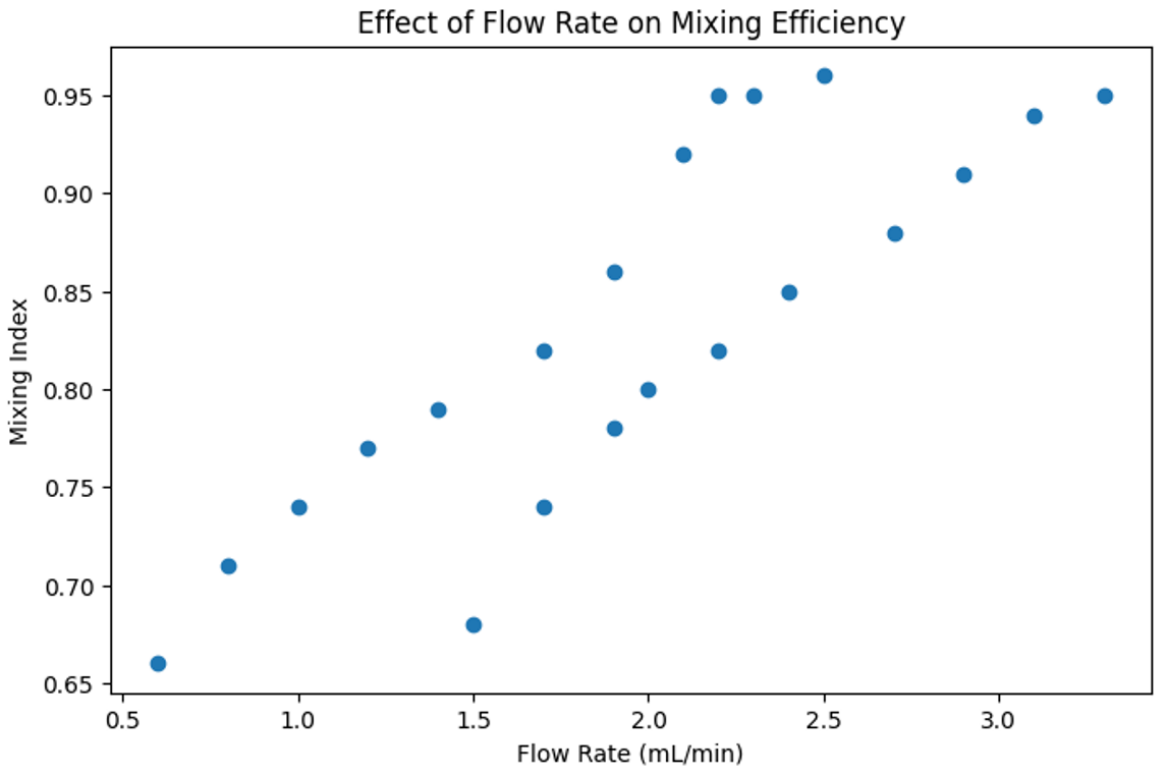

Figure 2. Variation of mixing index with flow rate for zigzag and split-flow micromixers.

3.1.3. Effect of Viscosity

The experimental observations in the split flow micromixer configuration showed that the mixing efficiency decreases with the increase of the fluid viscosity as can be seen in Figure 3. The mixing index fell gradually from around 0.94 at 1.5 mPa.s to around 0.70 at 6.5 mPa.s, showing a close inverse correlation between the viscosity and the mixing performance. The higher the viscosity of the fluid, the more viscous resistance it will have, which can be the reason for this decrease in mixing efficiency. In such a microchannel, the fluid homogenization is limited by the use of convective mixing mechanisms, which are also suppressed by higher viscosity. It should be noted that under constant flow rates, higher viscosity decreases the Reynolds number values which subsequently leads to lower inertial effects and less mixing enhancement. Previous experimental and machine-learning-assisted studies of fluid processing [3, 7] have reported similar viscosity-dependent decreases in micromixing performance. The present results thus demonstrate that the fluid viscosity is one of the key operational parameters that may affect the efficiency of the passive micromixer, and must be carefully taken into account when optimizing microfluidic systems.

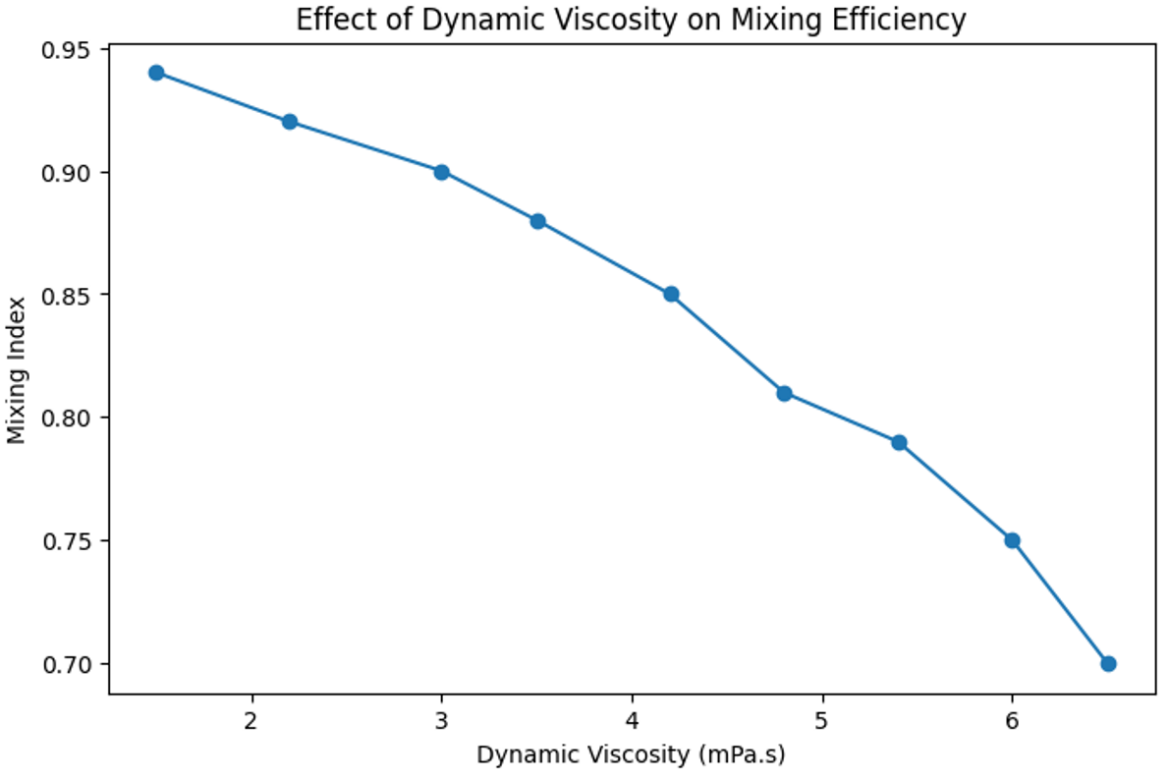

Figure 3. Effect of dynamic viscosity on mixing efficiency within the split-flow micromixer.

3.2. Machine Learning Performance

The three machine learning models trained using the experimental data set of the micromixer were: Linear Regression, Decision Tree Regressor, and Random Forest Regressor. The predictive ability of the models was assessed from RMSE and R^2 score. The model with the lowest RMSE value, 0.0207, and the highest R^2 score, 0.8827, was the Linear Regression model as shown in Table 1.

Table 1. Performance comparison of machine learning models for mixing-index prediction.

Model	RMSE	R^2 Score
Linear regression	0.0207	0.8827
Decision tree regressor	0.0543	0.1925
Random forest regressor	0.0389	0.5861

The R^2 is high and the model predicts a large percentage of the variation in the data set used for the experimental mixing-index. The low prediction error also indicates a good agreement between the predicted and experimental values of the mixing index. The Decision Tree Regressor model had the worst predictive power of all the models tested with an RMSE of 0.0543 and an R^2 of 0.1925. The relatively poor performance may indicate limited generalization ability and potential overfitting due to the small size of data sets and a lack of variability in the features. The Random Forest Regressor achieved moderate predictive performance with an RMSE value of 0.0389 and an R^2 score of 0.5861. The ensemble-learning approach increased the stability of predictions over the single Decision Tree model, but the Random Forest model was not found to be better than the simpler Linear Regression model.

The superior performance of Linear Regression indicates that the flow rate, Reynolds number, viscosity, geometry, and mixing index in the current dataset are reasonably linear. This observation is not unreasonable given the relatively small, structured and controlled nature of the experimental data. Other machine learning-based micromixer research has also demonstrated high prediction accuracy for regression-based surrogate models and optimization algorithms [6, 10, 11].

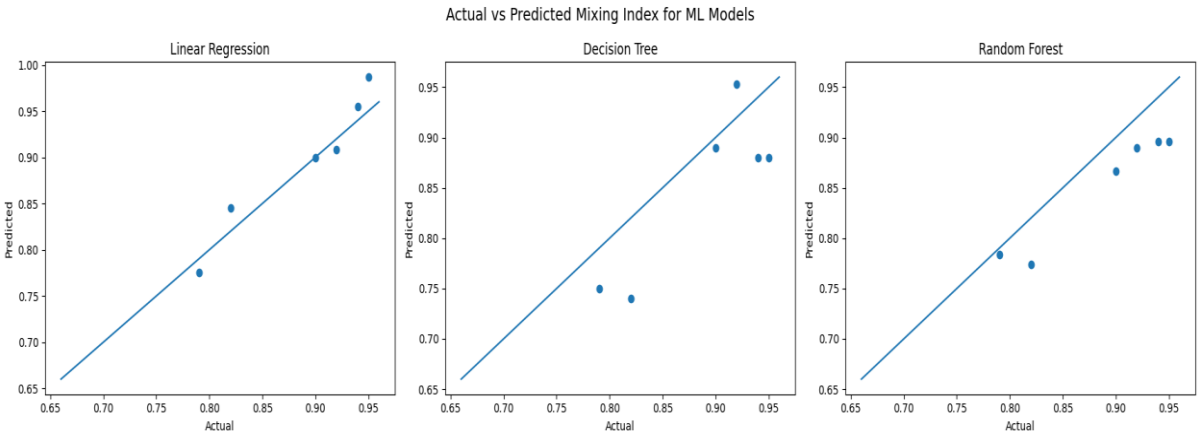

Figure 4. Actual versus predicted mixing-index values for the evaluated machine learning models.

Figure 4 illustrates the comparison between the actual and predicted mixing-index values for the evaluated machine learning models. It shows that the model of Linear Regression has the best agreement with the experimental data, which means that it has the highest predictive power.

3.3. Explainable AI Results

To assess the relative importance of the input variables for the prediction of mixing-index, feature-importance analysis and SHAP explainability analysis was conducted. As per the Table 2, the Random Forest feature importance analysis shows that flow rate was the most important predictor variable with the importance value of around 0.497.

Table 2. Random forest feature-importance ranking.

Feature	Importance
FlowRate_mL_min	0.4968
ApproxReynoldsNumber	0.3081
DynamicViscosity_mPa_s	0.1076
GeometryCode	0.0874

Figure 5 illustrates the Random Forest feature-importance ranking of the input variables used for mixing-index prediction. The second most influential variable was the Reynolds number with an approximated importance value of about 0.308, while the viscosity and the geometry had a low impact. The dominance of the flow rate and Reynolds number suggests that the operating flow conditions have a significant effect on the performance of the passive micromixer. The effects of increasing flow rate are to increase convective transport, interfacial stretching and chaotic advection, which all improve the efficiency of fluid mixing. In addition, Reynolds number affects the intensity of both the inertial mixing and the convective mixing in the microchannel. Figure 6 shows the summary plot of SHAP which explains the impact of all the inputs on the model predictions, and consequently on the estimation of mixing index. The positive effects of increased flow rate and Reynolds number on prediction of mixing-index was also confirmed by the summary analysis of the results from the SHAP. The higher the flow-rate value, the more positive the SHAP value was, which means that it was more efficient at predicting the mixing efficiency. On the other hand, higher viscosity values negatively affected model predictions, which is consistent with the previous conclusion that increasing the viscous resistance of the fluid reduces the mixing performance. The geometry variable had a moderate contribution to the model predictions. While geometry had an effect on mixing performance, this effect was relatively small compared to the effect of operational flow parameters since only two geometry classes were used and there was a limited variation in geometry between the classes.

The explainability results thus indicate that under the experimental parameters investigated, the flow-related parameters are crucial to the performance of the passive micromixer. The results are found to be in good alignment

with the previous explainable machine learning studies which highlighted the significance of operational variables on microfluidic mixing processes [1].

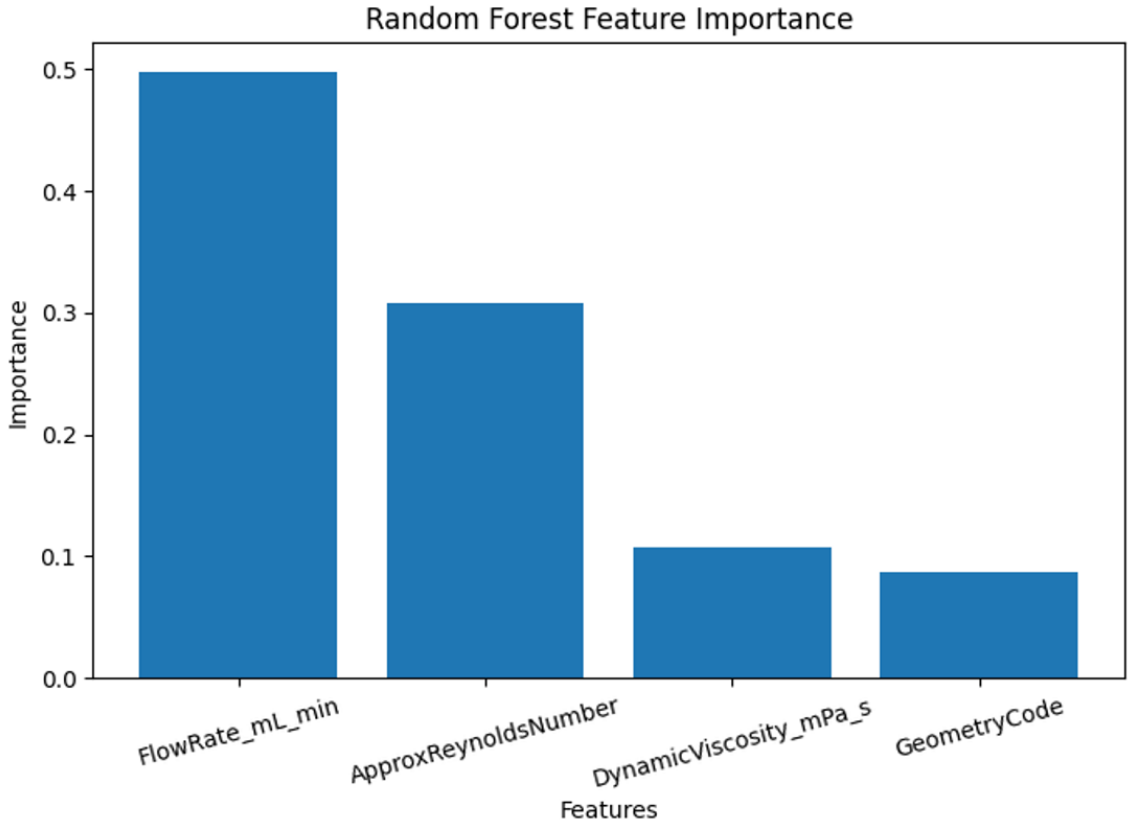

Figure 5. Random forest feature-importance analysis for mixing-index prediction.

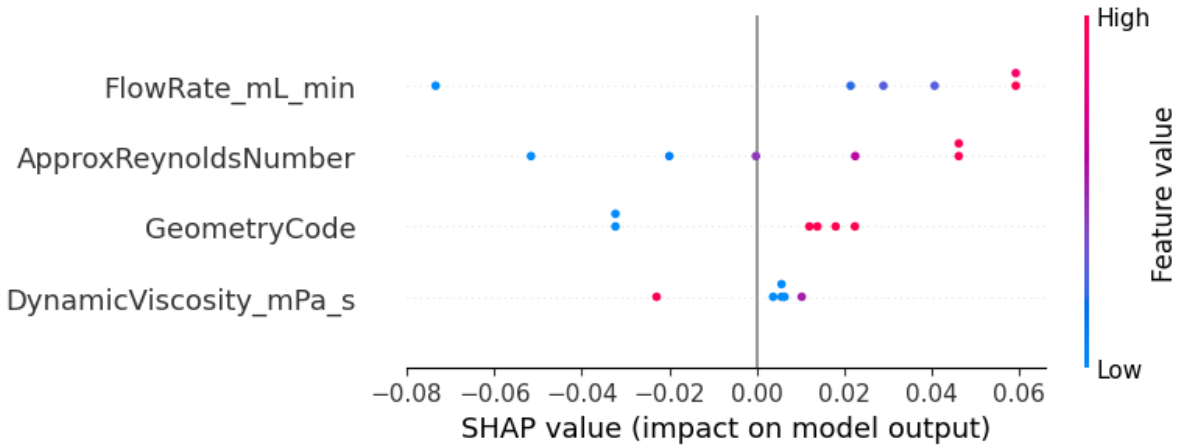

Figure 6. SHAP summary plot showing the contribution of input variables to mixing-index prediction.

3.4. Discussion

Based on the results of the experiments and the machine learning, the present study shows that the mixing efficiency of a passive micromixer can be well predicted by explainable machine learning approaches with the experimentally generated data. The Linear Regression model is more accurate for predicting the mixing efficiency, suggesting that the investigated operational and geometric parameters have relatively predictable relationships with the mixing efficiency under the studied conditions.

The dependency of mixing efficiency with flow rate and Reynolds number observed is well comparable with the classical passive microfluidic mixing theory. The flow rate increases can lead to an increase in the efficiency of interfacial stretching and diffusion inside the microchannel due to the stronger convective and chaotic advection. On

the other hand, higher viscosity decreases the chances of fluid deformation and limits the mixing enhancement mechanisms, which results in lower mixing efficiency values. The results of machine learning are broadly similar to previous studies using a neural network-based and an optimization-based micromixer. Maionchi, et al. [12] showed that artificial neural network (ANN) is an effective tool for predicting flow parameters and mixing behaviour of micromixer at different operational conditions. In the same way, McIntyre, et al. [13] reported that the optimized passive micromixer's geometry significantly enhanced the mixing performance by enhancing the flow-structure interaction. One approach that has proven to be effective for capturing complex microfluidic mixing behaviour with reduced reliance on conventional CFD simulations is the physics-informed neural-network approach [14]. The explainable AI analysis performed in the present study is more than just predictive accuracy; it offers engineering insight. Both the SHAP and feature-importance analyses showed that flow-related parameters were more influential in the mixing performance than geometry for the investigated dataset. This is reasonable, as the operational variables changed continuously throughout the experiments while only 2 geometry classes were examined. In recent passive micromixer studies based on clustering and optimization [15] similar prioritization of flow-related variables was reported. The present study shows that explainable machine learning frameworks can give efficient and interpretable alternatives to the repeated CFD simulations and experimental trial-and-error optimization in passive micromixer optimization from an engineering perspective. Thus, the experimental data incorporation, regression-based prediction, and explainable AI may serve as an exciting approach to speed up microfluidic device design and performance analysis.

The present results are in agreement with the recent progress in the field of passive micromixer research, where the mixing performance has been gradually enhanced by adopting geometry optimization and intelligent computational methods. Recent studies have demonstrated that structured micromixers improve nanoparticle synthesis and mixing efficiency [16], while planar micromixers with enhanced chaotic advection and bent baffles have achieved superior mixing through optimized flow structures [17], [18]. At the same time, surface-induced charge effects have been reported to improve micromixing in pressure-driven systems [19] and passive oscillating micromixers have been reported to further improve fluid interaction under laminar flow [20]. In a recent extensive review, it was confirmed that geometric optimization is still one of the most effective approaches to enhance passive micromixer performance in various applications [21]. In addition, optimized channel configurations of modified T-type micromixers, serpentine geometries and curved microchannels have all shown great potential improvements in mixing performance [22, 23, 24]. Recently, Bayesian optimization has been proposed as an efficient machine-learning method to speed up microfluidic design by decreasing the computational cost without sacrificing exploration of the complex space for microfluidic design [25]. The present results are backed up by these studies, in which an optimized micromixer design and a data-driven prediction are shown to offer an effective pathway for passive microfluidic systems to be improved.

4. CONCLUSION

This research presented an explainable machine learning model for predicting mixing efficiency of passive microfluidic micromixers based on experimentally obtained data. Experimental results showed that the geometry of the micromixer and the operating flow conditions were important factors affecting mixing. The mixing-index value was always greater for the split-flow micromixer than for the zigzag configuration, and higher flow rate and Reynolds numbers led to better mixing efficiency by promoting the convective transport and chaotic advection mechanisms. On the other hand, a more viscous fluid led to less mixing due to viscous resistance and less inertial effects. The three regression models were tested for their ability to predict the mixing index, which are Linear Regression, Decision Tree Regressor and Random Forest Regressor. Linear Regression was the model with the lowest RMSE and the highest R^2 score, suggesting that the experimental data set used in the study had relatively linear relationships between the selected variables. The Random Forest model showed a moderate predictability while the Decision Tree model had relatively poor generalization performance. Further explainable AI analysis also identified that flow rate

and Reynolds number were the most significant parameters for mixing-index prediction, with the viscosity and geometry having relatively lesser influences. The SHAP analysis and feature importance highlighted the relationship between operational conditions and the passive micromixer performance in a measurable and understandable way, enhancing transparency and understanding of the predictive framework. The results highlight the potential for novel passive micromixer analysis and prediction using explainable machine learning combined with microfluidic experimental data. The proposed framework offers a low computational cost and interpretable alternative to repeated experimental testing and optimization using CFD. The study therefore highlights the potential application of explainable machine learning methods in the design, optimization, and performance evaluation of passive microfluidic systems.

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Transparency: The author states that the manuscript is honest, truthful, and transparent, that no key aspects of the investigation have been omitted, and that any differences from the study as planned have been clarified. This study followed all writing ethics.
Competing Interests: The author declares that there are no conflicts of interests regarding the publication of this paper.

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