



Machine learning-assisted fracture prediction: integrating synthetic and experimental data for quasi-static notch failure analysis

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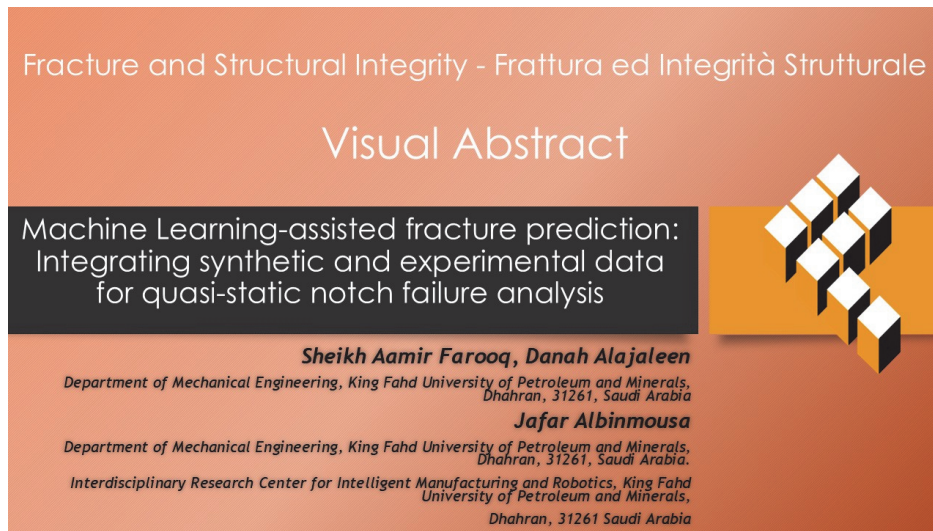
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Citation: Farooq, S. A., Alajaleen, D., Albinmoussa, J., Machine learning-assisted fracture prediction: integrating synthetic and experimental data for quasi-static notch failure analysis, Fracture and Structural Integrity, 75 (2026) 362-372.

Received: 28.09.2025

Accepted: 11.11.2025

Published: 23.11.2025

Issue: 01.2026

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KEYWORDS. Machine Learning, Fracture, Theory of Critical Distances, PYMAPDL, Synthetic data, XGBoost.

INTRODUCTION

Polycarbonate (PC) is a high performance thermoplastic that possesses high impact resistance, excellent mechanical strength, making it suitable for high impact applications [1,2]. In addition, polycarbonate exhibits transparency due to its non-crystalline structure; nevertheless, it is almost as strong as highly crystalline nylon and is even tougher [3]. The superior mechanical and physical properties of polycarbonate have led to its widespread use in various industries including automotive [4], medical [5], aerospace [6], construction [7] and electronics [8]. Given the increasing demand in



these diverse applications, particularly in load-bearing components, it is important to understand the fracture behavior under various loading conditions, especially when geometrical discontinuities such as notches or cracks are present.

Notches and other defects are often inherent due to design limitations, manufacturing processes or in-service damage. Geometrical discontinuities act as stress concentrators and potential crack initiation sites, which create complex stress and strain distributions near the notch tip, thereby complicating the fracture prediction. Consequently, it is essential to have a reliable design methodology for predicting the fracture load on notched members [9]. Traditional fracture mechanics methods often fall short in capturing the fracture behavior of notched ductile polymers such as polycarbonate under quasi-static loading [10]. Numerous continuum-mechanics based constitutive models have been developed over recent decades to describe the complex mechanical behavior of polycarbonate, accounting for viscoplastic behavior and notch sensitivity [11–13]. While these models significantly enhance predictive accuracy, they require extensive experimental calibration and computational effort. Therefore, alternative methods such as Theory of Critical Distances (TCD) [14] and Strain Energy Density (SED) [15] have gained significant attention to estimate the fracture of different notch geometries and materials, without the need for extensive crack growth modeling.

Among these methods, TCD is most widely used due to its simplicity for accurate fracture prediction in notched members. Among its various formulations, the point method of TCD (TCD-PM) has been particularly favored due to its ease of implementation and low computational cost. TCD has been successfully applied to a wide range of materials and notch geometries, estimating fracture under quasi-static and dynamic loading conditions [16–18]. Another important aspect of TCD is its ability to predict fracture accurately without requiring non-linear material modelling or complex computational analyses. Nonetheless, TCD still depends on accurate stress fields obtained from finite element analysis and requires experimental data to calibrate its parameters. Conducting fracture experiments across a wide range of geometrical configurations can be costly and time-consuming, particularly for ductile materials like polycarbonate. Additionally, experimental techniques such as Digital Image Correlation (DIC), also add to complexity and cost of the experimental testing [19].

In recent years, data driven approaches based on Artificial Intelligence (AI) and Machine Learning (ML) have emerged as powerful techniques for predictive modeling in fracture mechanics. ML algorithms have shown exceptional capabilities in capturing complex non-linear relationships and making accurate predictions even with limited input data. Recently, many ML models, such as decision trees, random forests, support vector machines (SVM), and gradient boosting frameworks like XGBoost have shown great promise in predicting fracture and fatigue in various engineering materials [20,21]. Moreover, the use of synthetic datasets generated from finite element simulations have been used for the training of different ML models, reducing the need for extensive experimental data and testing. Aldakheel et al. [22] developed a physics-based ML framework trained on synthetic dataset generated from finite element-based phase-field fracture simulations to predict both brittle and ductile fracture. Similarly, Xu. et al., proposed Crack-Net, which uses phase-field simulation data to train a deep learning model that predicts crack propagation in composite materials [23]. Further, Mocerino et al., [24] trained a surrogate ANN model using synthetic data generated with the cohesive crack-finite element model, to estimate fracture parameters in translaminar fracture of structural composites. These studies demonstrate that use of synthetic datasets in ML training is becoming a practical route to reduce dependency on expensive experimental testing.

This study aims to combine the synthetic datasets generated using TCD-PM with experimental data to train an XGBoost machine learning model for predicting the quasi-static fracture behavior of notched polycarbonate specimens. Experimental data is reduced systematically and replaced with synthetic data to analyze the predictability of the model minimizing experimental testing.

MATERIALS AND METHODS

Materials and specimen preparation

The material used in this study is Polycarbonate (PC). A PC sheet with dimensions of 3000 mm in length and 2050 mm in width and thickness 6 mm was sourced from Rowad National Plastic company, Saudi Arabia. The properties of the PC sheet provided by the company are summarized in Tab. 1.

Modulus of Elasticity	Tensile Strength	Elongation at Yield	Elongation at Fracture
2400 MPa	58 – 60 MPa	6 %	110 %

Table 1: Properties of PC sheet (as provided by the manufacturer).

Standard tensile and U-notched rectangular specimens were cut from this PC sheet. The tensile specimens were machined as per ASTM D638-22 standard [25], with dimensions as shown in Fig. 1. A total of eleven U-notched samples with varying notch depths (d_p) and notch radii (ρ) were prepared as rectangular plates measuring 210 mm in length and 26 mm in width, as illustrated in Fig. 2.

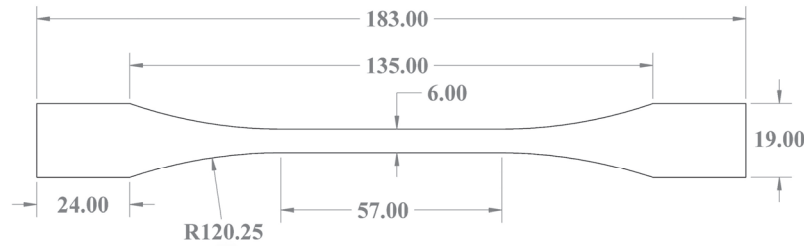


Figure 1: Tensile Specimen. All dimensions are in mm.

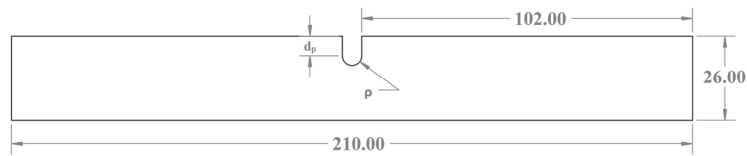


Figure 2: U-notched specimens. All dimensions are in mm.

Experimental testing procedure

The mechanical tests were conducted under quasi-static loading conditions on Instron 5569 universal testing machine equipped with a 50 kN load cell. All tests were performed at a constant displacement rate of 5 mm/min. The tensile tests were performed on five specimens and strain was measured using two independent systems: a clip-on extensometer and a Digital Image Correlation system. The fracture experiments on U-notched specimens were conducted to determine the fracture load for eleven different configurations with notch depths ranging from 4 mm and 7 mm and notch radii between 1.5 mm and 5 mm. Three duplicates were tested for each configuration to ensure reproducibility. DIC was used for selected samples to visualize and quantify the strain field near the notch tip.

Determination of TCD parameters

The Theory of Critical Distances-Point Method (TCD-PM) was used in this study to estimate the fracture in the U-notched specimens. TCD-PM assumes that fracture occurs when the stress at a certain distance from the notch tip, known as critical distance, reaches a material-dependent critical value [14]. The critical distance ($L/2$) can be calculated using the material's fracture toughness and inherent strength using Eqn. 1.

$$L = \frac{1}{\pi} \left(\frac{K_{IC}}{\sigma_0} \right)^2 \tag{1}$$

The critical distance and the inherent strength can also be calculated experimentally for materials exhibiting plastic behavior. The inherent strength and critical distance have been determined in our previous works [9,26] by examining the principal stress distribution ahead of notch tip for varying notch geometries and identifying the intersection point of their stress-distance curves. The values for critical distance ($L/2$) and inherent strength (σ_0) were found to be 6.95 mm and 54.5 MPa, respectively. These constants were used in all subsequent fracture predictions in finite element simulations based on point method, as described in following sections.

Finite element modeling and fracture load predictions

A linear elastic element model was developed in ANSYS Mechanical via PyMAPDL to simulate the U-notched specimens and extract stress values for TCD-PM calculations. As already mentioned, TCD-PM is based on linear elastic analysis, so the material behavior of polycarbonate was assumed to be linear elastic with Young's modulus and Poisson's ratio equal to 2267.6 MPa and 0.38, respectively [26]. Although polycarbonate exhibits elastic-plastic behavior under large deformation, the use of a linear-elastic material model was adopted to maintain consistency with the theoretical basis of TCD-PM



approach, which evaluates fracture initiation from elastic stress distribution at a defined critical distance from the notch-tip. Experimental results discussed in result section showed that fracture initiation coincides with the onset of necking, where the local stress field can still be approximated as linear elastic. Therefore, adapting a linear-elastic material model ensures consistency between the experimental fracture load and TCD-PM predictions, as also reported in previous studies [9,26]. The geometry was modeled as a 2D plane stress with thickness with actual specimen dimensions, however only half the specimen was modeled due to symmetry of the specimen. The geometry was meshed using Plane 183 elements with refined meshing near the notch tip as shown in Fig. 3. For the boundary conditions, the displacement was restricted in the vertical direction at the lower edge of sample and in the horizontal direction at the edge of the geometry. The load was applied as a negative pressure at the top edge to simulate quasi-static loading [26]. Fracture loads were calculated for the eleven specimens by incrementally applying the load and calculating the stress at the critical distance (6.95 mm) with the inherent strength of the material (54.5 MPa). The load at which the stress is equal to inherent strength was taken as fracture load for that geometry.

Synthetic dataset generation using PYMAPDL

The synthetic dataset used in the machine learning model was generated using PYMAPDL by varying the notch depth and notch radius. A total of 32 synthetic data points were produced with notch radii ranging from 1.5 mm to 4.5 mm, and depths from 4.5 mm to 10 mm, without overlapping the experimental specimen geometries. The same finite element analysis setup and material model were employed. A looped simulation was implemented where the load gradually increased in steps of 50 N, and the maximum principal stress at critical distance was extracted at each step, until it reaches or exceeds the inherent strength value of 54.5 MPa. If the stress exceeds this value, the routine fine-tunes the load steps to 5 N and then to 1 N, running the simulation from the last load which corresponds to stress below inherent strength, until it reaches the value of 54.5 MPa to accurately determine the fracture load. The final load where the maximum principal stress at the critical distance (6.95 mm) equals inherent strength (54.5 MPa) was recorded as the predicted fracture load for that specific geometry. This method generates high-fidelity synthetic dataset linking the notch depth and radius to predicted fracture loads, which was later used for the training and validation of the machine learning model as discussed in the following section. It is important to mention that the synthetic dataset generated is valid within the geometric and material assumptions inherent to finite element model. The notch radius (ρ) and depth (d_p) combinations were varied between 1.5 to 4.5 mm and 4 to 10 mm, respectively as it was observed when the notch radius or depth exceeds certain limits, the geometry could not be meshed. Therefore, the synthetic data are considered valid and acceptable only within the range mentioned, maintaining the same specimen thickness, boundary conditions. The simulations remained stable and consistent with the experimental configurations in this range. Moreover, the TCD-PM assumes linear-elastic stress fields, these results are applicable only up to the onset of fracture-initiation under quasistatic loading. Thus, extrapolation beyond these geometric or material limits, may introduce increasing uncertainty. The present model thus defines a bounded synthetic domain suitable for augmenting experimental data in quasi-static tensile loading of U-notched polycarbonate specimens. \dot{U}

Machine Learning framework

In this study, XGBoost (Extreme Gradient Boosting), a ML boosting algorithm for regression by Chen and Guertin [27] was used for its robust performance in regression problems, particularly in handling small and medium datasets with non-linear dependencies. XGBoost combines the predictions to arrive at a final prediction which is the sum of the predictions of all weak learners. XGBoost has an inbuilt capacity for regularization and avoids overfitting [28].

The model was trained using combinations from the 33 experimental points (three duplicates for each of the 11 geometries) and 32 synthetic data points. The input features were the notch radius and notch depth, while the target variable was fracture load. A total of six combinations were tested including experimental-only data (22), hybrid combinations (e.g., 75% exp + 25% synth, 50% exp + 50% synth., 25% exp + 75% synth.), synthetic only, and finally a full-dataset. A fixed set of 11 experimental specimens was used across all models for testing to ensure a valid comparison. In hybrid combinations, the experimental data points were progressively replaced with randomly selected synthetic data points sampled from a pool of 32 unique geometries, not present in the experimental data set, as per the percentage of synthetic data used in each model. The total number of points was kept constant at 22 in all models to ensure consistency across models. To ensure consistent validation, 11 experimental specimens were randomly selected and fixed as the test dataset across all models. These points were excluded from all training sets, including the full-dataset model, which used 22 experimental and 32 synthetic data points for training. This ensures validation of the ML models by ensuring that testing was always performed on unseen geometrical geometries. Tab. 2 summarizes the training and test dataset compositions, evaluation metrics, and XGBoost parameters adopted for all configurations.

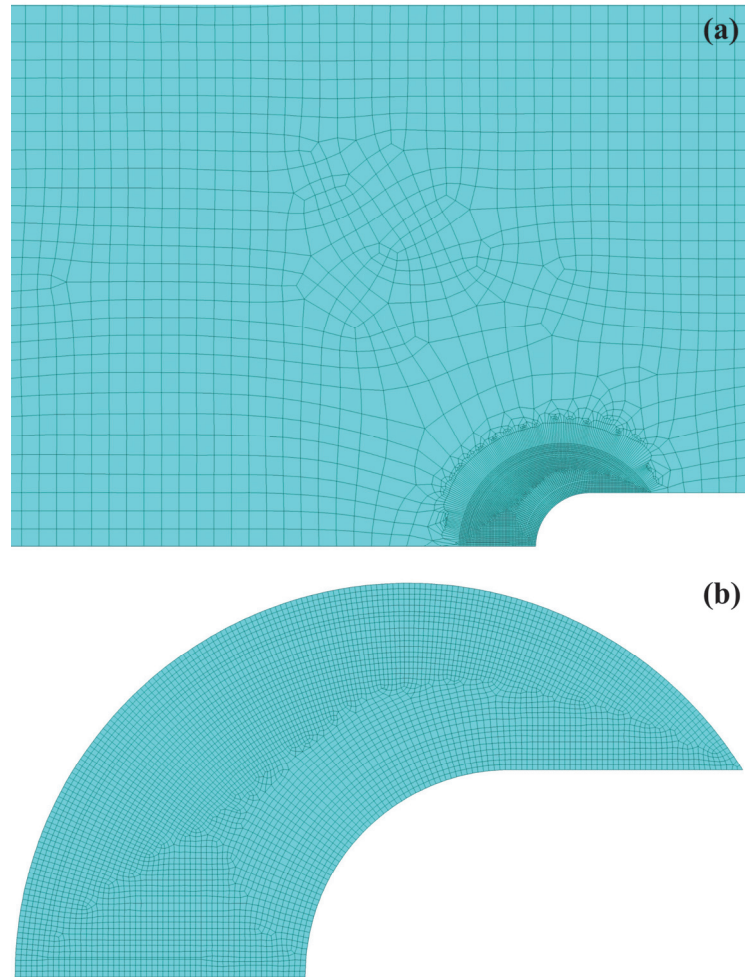


Figure 3: (a) View of the general mesh and (b) Refined mesh around notch area.

Model	Training Data Composition (Total=22)	Test Data (Fixed)	Evaluation Metrics Used	XGBoost Parameters	Purpose
Exp-only	22 Experimental				Baseline reference model
75 % Exp + 25 % Synthetic	16 Experimental + 6 Synthetic				Evaluate effect of limited synthetic data
50 % Exp + 50 % Synthetic	11 Experimental + 11 Synthetic	11 Experimental (Fixed across models)	MAPE, MAE, RMSE, R ²	n_estimators = 500, learning rate = 0.01, max depth = 5, random state = 39	Hybrid dataset with balanced composition
25 % Exp + 75 % Synthetic	6 Experimental + 16 Synthetic				Synthetic-dominant composition
Synthetic only	22 Synthetic				Evaluate synthetic-only generalization
Full Dataset (Exp + Synthetic)	22 Experimental + 32 Synthetic				Combined model for maximum robustness

Table 2: Summary of XGBoost model training and validation setup

The XGBoost regressor was configured with 500 $n_{estimators}$, a learning rate of 0.01 and maximum tree depth of 5. These parameters were selected to ensure stable convergence and avoid overfitting, especially given the relatively small dataset size. In addition, to ensure consistency in results, each model was trained using the same random state (39) and number of data points (22 for training) with only the composition of experimental and synthetic data varying between them. The only exception being the full dataset model which used all 54 data points for training. The model performance was evaluated using standard regression metrics including Mean Absolute Percentage Error (MAPE), Root Mean Square Error (RMSE), Mean Absolute Error (MAE) and Coefficient of Determination (R^2).

RESULTS AND DISCUSSION

Tensile specimen test results

The stress-strain curve from the tensile testing of polycarbonate specimens using both an extensometer and Digital Image Correlation (DIC) is presented in Fig. 4(a). The stress-strain curves obtained from the extensometer and DIC system show good agreement up to the necking point. The tensile behavior of the specimen is comprehensively discussed in our previous works [9,26]. The typical tensile behavior for polycarbonate can be seen in the load-displacement curve for one of the specimens, illustrated in Fig. 4(b).

From the figure, a sudden drop in the load can be seen at Point A, which corresponds to the necking of the material. After the drop, the material continues to deform with growth of a plastic band until complete failure. However, necking point itself is considered as the failure point, which provides a consistent point of comparison for experimental results with TCD-PM which is based on a linear-elastic assumption. The average mechanical properties obtained from tensile tests are summarized in Tab. 3.

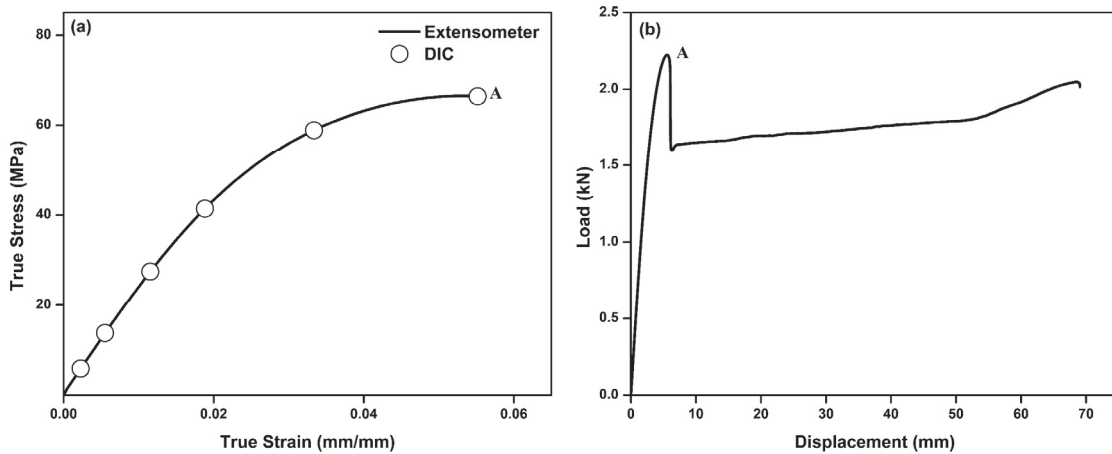


Figure 4: (a) True stress-strain curve obtained with DIC and extensometer, and (b) Load Displacement curve. Point A corresponds to beginning of necking.

Property	Average Value	Standard Deviation
Young's Modulus (E)	2267.60 MPa	47.01
Yield Stress ($\sigma_{0.2}$)	36.1 MPa	1.96
Yield Strain ($\epsilon_{0.2}$)	0.0177	0.0013
Necking Stress ($\sigma_{necking}$)	66 MPa	0.59

Table 3: Average mechanical properties of polycarbonate specimens from tensile test.

Fracture Behavior of U-notched Specimens

The fracture behavior of polycarbonate U-notched specimens was investigated under quasi-static tensile loading with specimens being loaded until complete failure. A detailed discussion of the failure mechanisms has been presented in our previous work [9]. In this section, we briefly summarize the key findings in the fracture of U-notched specimens.

Based on the nominal stress versus extension curves presented in Fig. (a) and 5(b) respectively, two distinct fracture modes can be observed, which are thoroughly discussed in [9]. In sharper notches such as those with $\rho = 1.5$ mm, failure occurs after the maximum load is reached without a significant drop in the load. Consequently, in specimens with larger radius



such as $\rho = 5$, $d_p = 6$, a noticeable drop of about 8 % in the load can be seen after peak stress, as illustrated in Fig. 5(a). Similar behavior was noticed for specimens with $\rho = 3.5$ mm and $d_p = 6$ mm. The experimental fracture loads for each geometrical configuration are given in [9]. Those results are used in subsequent sections for evaluating the accuracy of TCD-based and machine learning fracture predictions.

Fracture load prediction using the Theory of Critical Distances (TCD-PM)

The fracture loads of notched polycarbonate specimens were estimated based on TCD-PM formulation. As mentioned previously, the fracture load is predicted by the finite element simulation using PYMAPDL by comparing the maximum principal stress at critical distance of 6.95 mm from notch tip with the inherent strength (54.5 MPa) of the polycarbonate. The predicted loads for all eleven experimental notch geometries were compared with the experimentally determined average fracture load, are summarized in Tab. 4 along with the percentage deviation.

The results show that the TCD-PM-based fracture load predictions show close agreement with the experimental data with discrepancies within ± 5 % (between -3.48 % and 4.40 %). This validates the applicability of TCD-PM method for fracture prediction in notched polycarbonate specimens under quasi-static loading. The consistency between simulation results and experimental data also indicates that fracture load data generated from PYMAPDL can be used as a reliable input for data-driven modeling approaches.

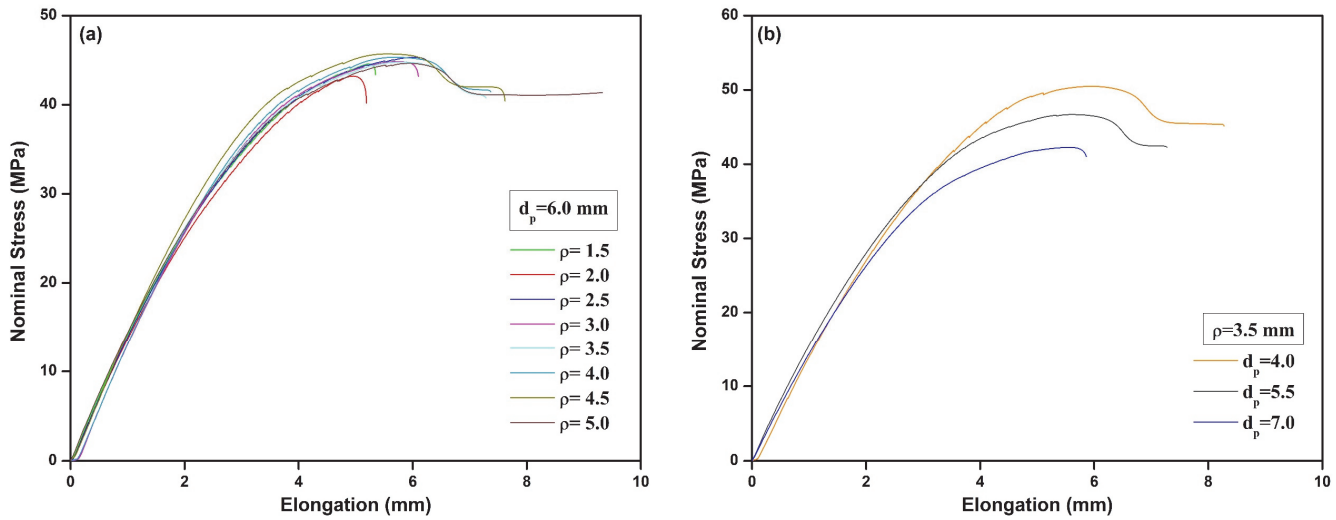


Figure 5: (a) Stress-Elongation curves for specimens with $d_p=6$ mm and different ρ , and (b) for specimens with $\rho= 3.5$ mm and different d_p .

ρ	d_p	Average Experimental Fracture Load, N	TCD-Predicted Fracture Load, N	Percentage Error
1.5	6	6885.8	6893.2	0.11
2	6	6703.8	6832.6	1.92
2.5	6	7018.3	6774.4	-3.48
3	6	6798.4	6718.7	-1.17
3.5	6	6637.3	6665.5	0.42
4	6	6448.8	6614.8	2.57
4.5	6	6499.7	6566.6	1.03
5	6	6427	6520.8	1.46
3.5	4	7054.3	7364.3	4.39
3.5	5.5	6582.3	6827.6	3.73
3.5	7	6591	6377.3	-3.24

Table 4: Estimated fracture load using TCD-PM Method, with percentage deviation from actual average experimental fracture load.

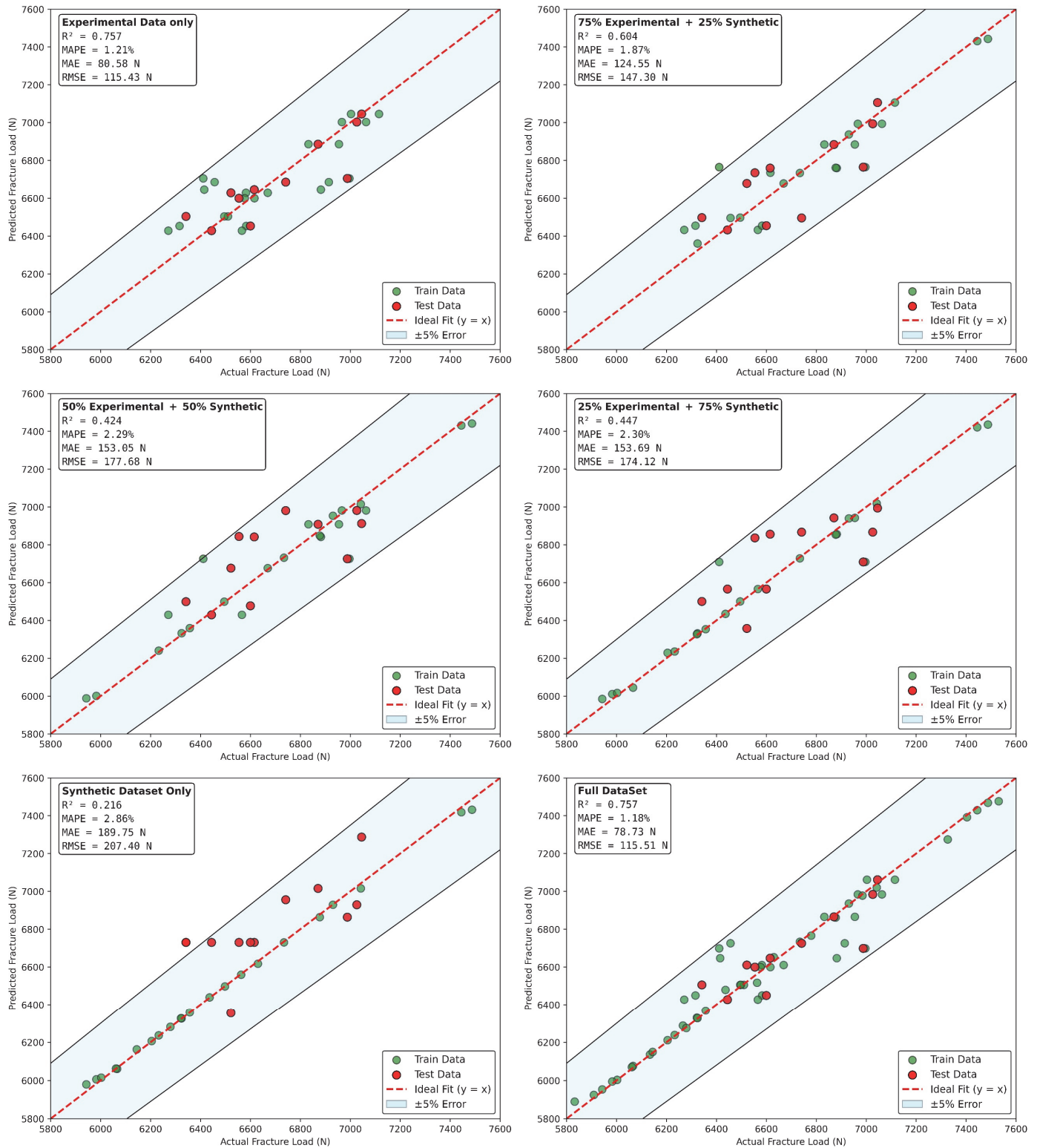


Figure 6: Predicted vs. actual fracture load plots for training and test data across six machine learning models trained on different combinations of experimental and synthetic data. The shaded region indicates a $\pm 5\%$ error band around the ideal prediction line.

Performance of ML models for fracture load prediction

The XGBoost models were trained to evaluate the effect of the synthetic data on the model accuracy and robustness in predicting the fracture loads of U-notched polycarbonate specimens. Fig. 6 presents the actual vs. predicted for all six different models with R^2 , MAPE, MAE, and RMSE, shown for each model. The model trained purely on 22 experimental



data points demonstrated the most consistent alignment with the ideal fit line, achieving the lowest prediction error (MAPE = 1.23%) and high accuracy. As the percentage of the synthetic data increases in the hybrid models (25%, 50% and 75%), test accuracy decreases. This is because the training set has decreased noise and variability present in experimental-only model, leading to reduced generalization accuracy. The model trained on 22 synthetic data points only (randomly chosen from the synthetic dataset) fits its training data almost perfectly, given the deterministic nature of the synthetic dataset generated using TCD-PM, which lacks experimental irregularities. However, this model performed the lowest in terms of test accuracy and other test metrics and showed significant scatter on test points, as shown in Fig. 6. The model which combined all remaining experimental data points (22) and synthetic dataset (32 points), showed excellent performance, nearly identical to the experiment-only model. All the predictions are well within the $\pm 5\%$ errors as shown in Fig. 6.

The standard regression metrics for all six training compositions are presented in Fig. 7, which highlights that the full dataset training composition achieved the lowest MAPE (1.18 %) and MAE (78.83 N) across all models, while yielding a similar R^2 value. It is worth noting that R^2 score fluctuated significantly across all models, which is expected due to the small size of test set and its sensitivity to random sampling of training data, especially in hybrid combinations. Even though a fixed random state was used in all models, the random sampling of training data still leads to noticeably different R^2 values; however, accuracy as reflected by other metrics remains high and stable. Due to this reason, MAPE, MAE and RMSE were prioritized for evaluating performance and robustness of the models. Overall, the full dataset model was the best model in predicting the fracture loads of U-notched polycarbonate specimens. Tab. 5 summarizes the predicted fracture load from the XGBoost model using the full dataset, the experimental test loads and the discrepancy for eleven experimental test data points. The results show that the predicted fracture load from XGBoost ML model shows close agreement with the experimental data with discrepancy ranging from only -4.14 % to 2.59 %. This indicates synthetic data can significantly complement experimental data, thereby improving the robustness of machine learning models.

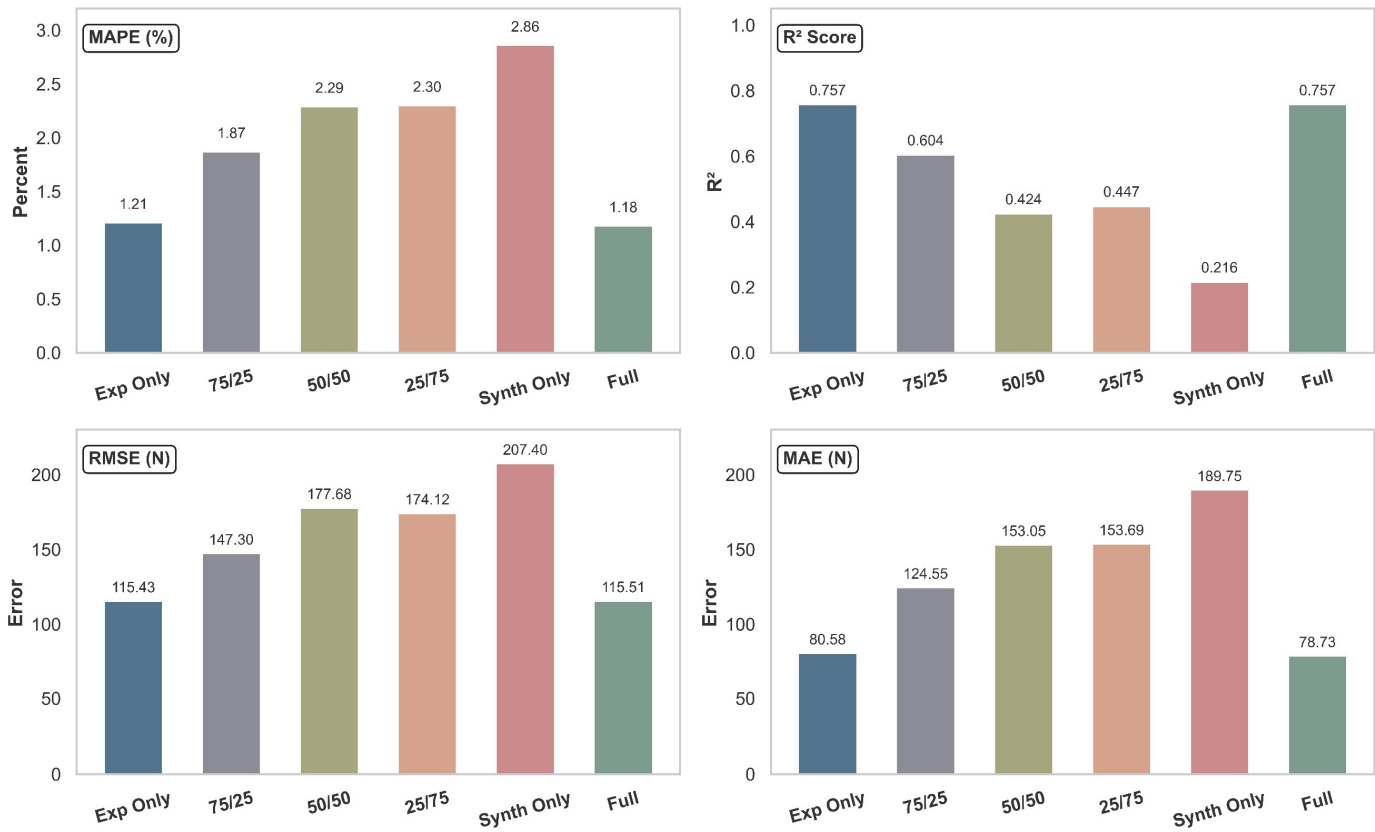


Figure 7: Performance comparison of six machine learning models trained on varying combinations of experimental and synthetic data.



ρ	d_p	Experimental Fracture Load, N	ML-Predicted Fracture Load, N	Percentage Error
1.5	6	6870.6	6865.826	-0.07
2	6	6741	6725.73	-0.23
2.5	6	7026	6984.101	-0.60
3	6	6988.1	6698.816	-4.14
3.5	6	6614.9	6646.832	0.48
4	6	6341.5	6505.538	2.59
4.5	6	6600	6449.638	-2.28
5	6	6444	6427.098	-0.26
3.5	4	7045	7062.107	0.24
3.5	5.5	6554	6599.902	0.70
3.5	7	6522	6610.532	1.36

Table 5: Estimated fracture load using XGBoost for full dataset compared with experimental test data.

CONCLUSION

In this study, a fracture mechanics and machine learning approaches were used to predict the quasi-static fracture load of U-notched polycarbonate specimens based on geometric features. Predictions from TCD-PM method showed close agreement with the experimental results. Further, a novel machine learning framework was developed using XGBoost regression model to predict the fracture loads based on notch geometry. The XGBoost regression models were trained with varying combinations of experimental and synthetic data generated using TCD-based PyMAPDL simulations. The results showed that among all combinations, the model trained with full dataset of experimental and synthetic data points achieved the best performance with a MAPE of 1.18 %, R^2 of 0.757 and MAE of 78.73 N only. Hybrid models using limited experimental data supplemented with synthetic data also demonstrated reasonable accuracy. The findings indicate that synthetic data can significantly reduce the need for testing and experimentation, although it cannot fully substitute for experimental validation, particularly in critical applications. Future work will extend this framework to new geometrical configurations and loading conditions (mixed mode) to further assess its generalization capability.

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NOMENCLATURE

ρ	Notch radius
d_p	Notch depth
σ_0	Inherent Strength of material