Modeling of Necking Area Reduction of Carbon Steel in Hydrogen Environment Using Machine Learning Approach

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Introduction

- Natural gas transport favors low carbon and alloy pipelines for their cost-effectiveness, weldability, longevity, and strength.
- Repurposing gas pipelines for hydrogen: Address regulatory, safety, and HE challenges.
- Addressing HE in Pipelines: Traditional mitigation strategies face adaptation challenges:
  - **Specialty Alloys**: Efficient, yet require costly specialized production.
  - **Protective Coatings:** Offer barriers, but come with expense and infrastructure modifications.
- Evaluating steel's embrittlement is resource-intensive; machine learning offers a more efficient, cost-effective solution.

Fig. 1: A 3D rendering of a hydrogen pipeline (Tez, S., et. al (2022)).

Objectives

- Utilize ML to analyze hydrogen behavior in low carbon and low-alloy steels under high pressures.
- Evaluate several ML techniques to best predict HE's impact on mechanical properties, especially reduction in area.
- Provide guidance on material selection for hydrogen pipeline construction based on steel behavior in hydrogen environments.

Methodology

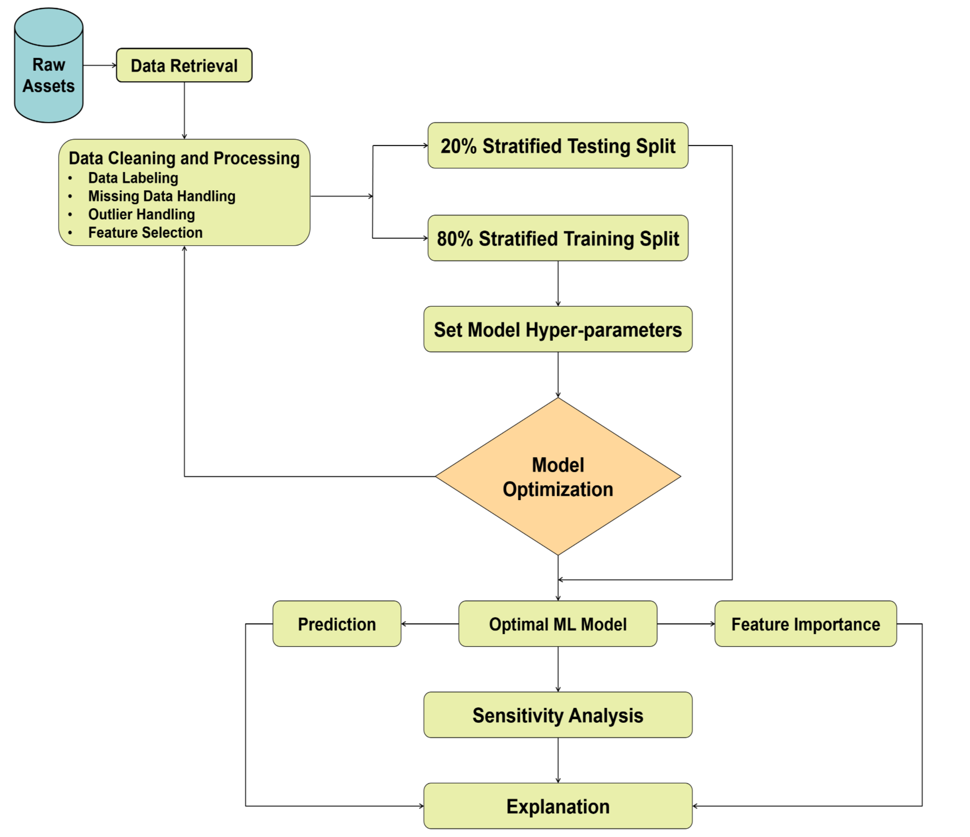


Fig. 2: Framework for Data Collection, Preparation, and Analysis.

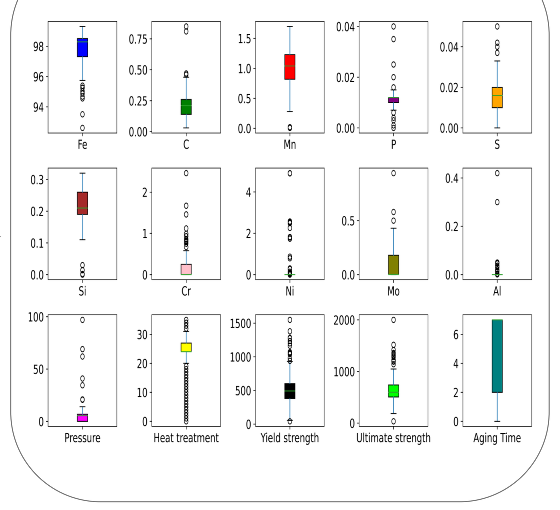
Results and Discussions

Data Processing

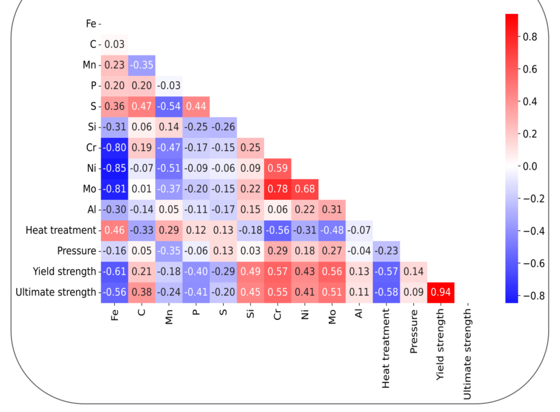
Database Summary

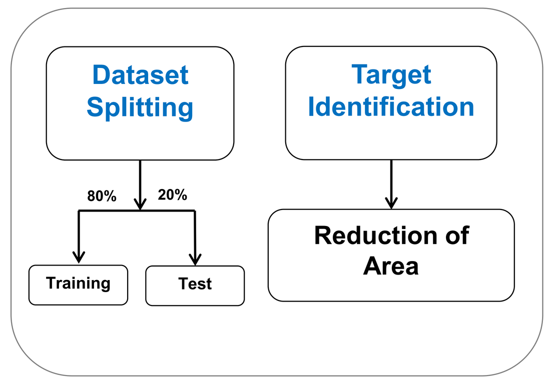
Categories	Parameters	Data Range (Minimum/Maximum)	Mean	Standard Deviation	Units
Chemical Properties	Iron (Fe)	92.61/99.31	97.812	1.131	%
	Carbon (C)	0.03/0.85	0.218	0.145	%
	Manganese (Mn)	0.007/1.70	1.025	0.352	%
	Phosphorous (P)	0.00/0.04	0.012	0.006	%
	Sulfur (S)	0.00/0.05	0.016	0.010	%
	Silicon (Si)	0.00/0.32	0.188	0.094	%
	Chromium (Cr)	0.00/2.46	0.266	0.455	%
	Nickel (Ni)	0.00/4.91	0.264	0.763	%
	Molybdenum (Mo)	0.00/0.94	0.087	0.156	%
	Aluminum (Al)	0.00/0.42	0.013	0.058	%
Mechanical Properties	Yield Strength (Su)	41.40/1550	529.95	249.764	MPa
	Ultimate Strength (Sy)	35/ 2000	653.047	256.539	MPa
	Reduction of Area (RA)	6.50/96.00	55.489	18.626	%
Test Conditions	Aging Time	0.00/7.00	4.852	2.971	Day
	Hydrogen Partial Pressure	0.10/97.00	13.125	23.246	MPa
	Strain Rate	2e-6/8e-3	2.43e-4	7.30e-4	s^{-1}
	Heat Treatment	Different heating treatment	-	-	-
	Product Form	Various sources*	-	-	-
	Hold Stress	0.00/9.00	6.483	3.059	MPa

Outlier Handling



Feature Selection





Machine Learning Model

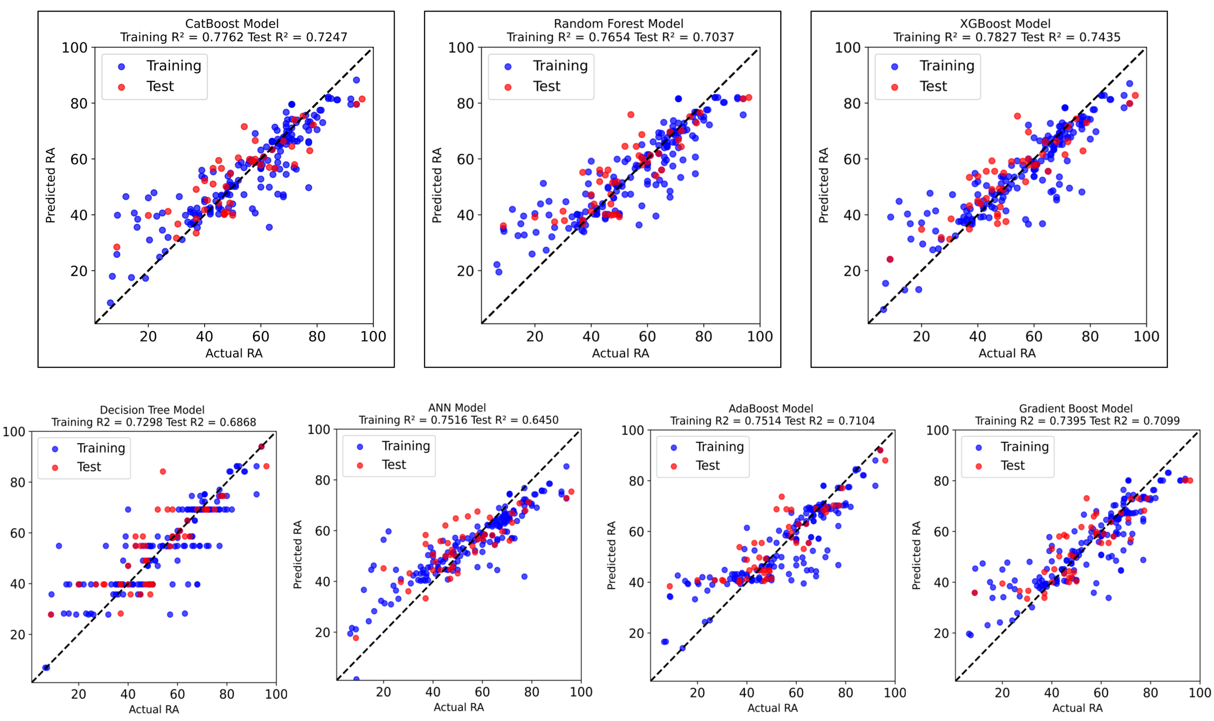


Fig. 3: Comparison of correlations between Actual RA and Predicted RA of seven ML models

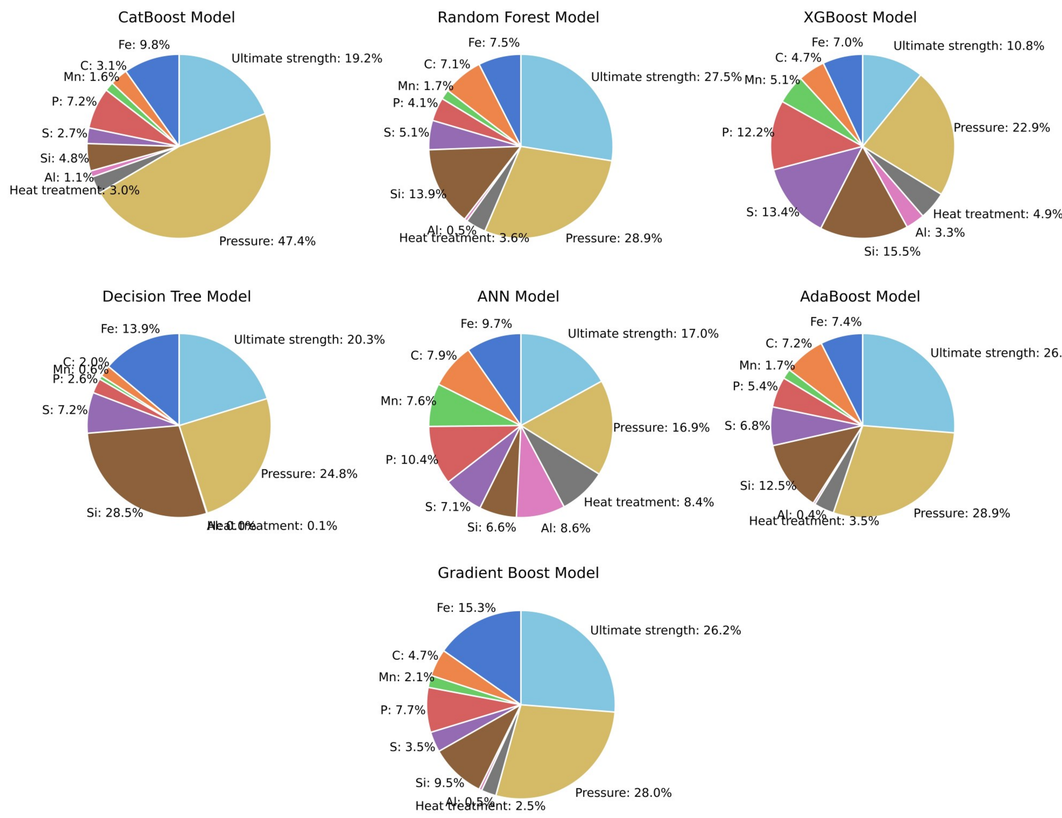


Fig. 4: Comparison of different features in predicting reduction of area using seven machine learning models

Performance Evaluation

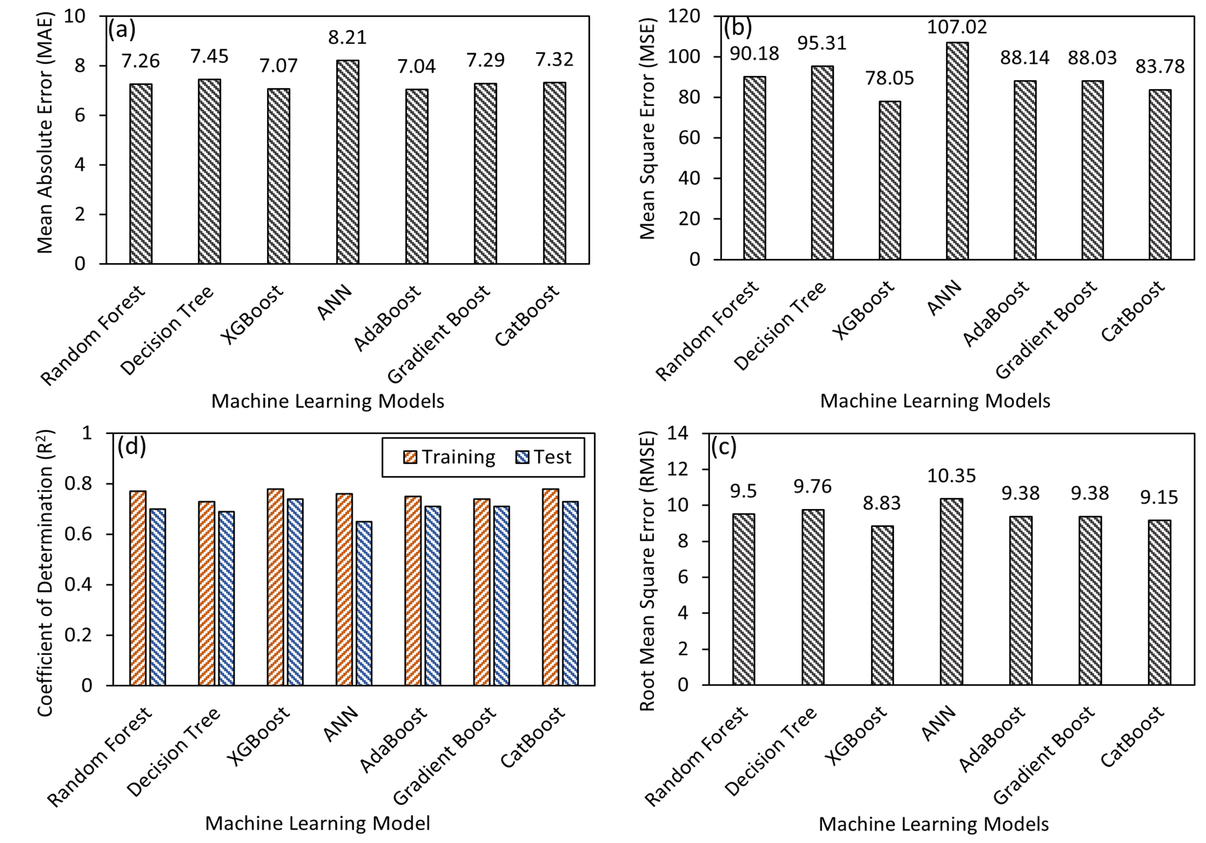


Fig. 5: Comparison of ML models performance based on (a) MAE, (b) MSE, (c) RMSE, and (d) R2

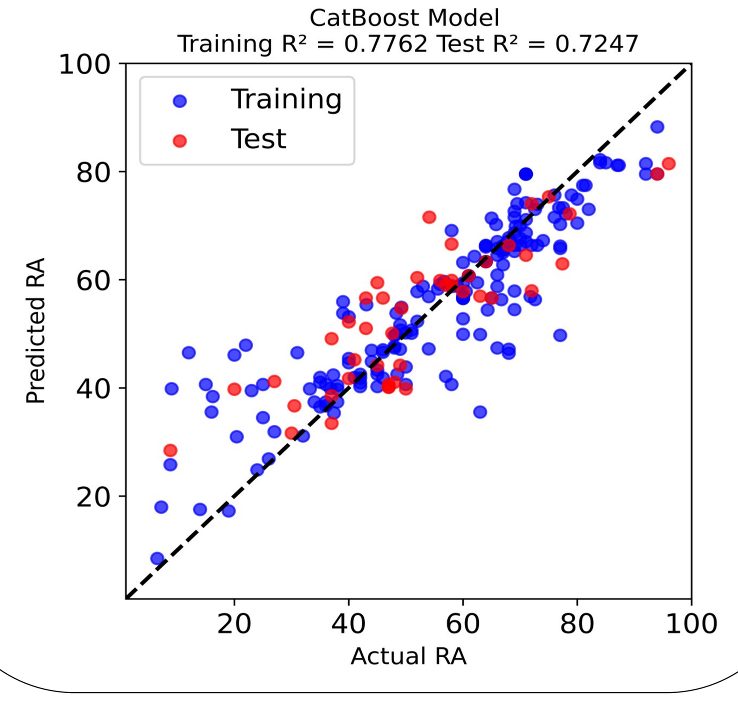
Optimum Model Selection

Model Name	Coefficient of Determination		MSE	RMSE	MAE	Pressure	Su	Fe	C	Si	S	P	Al	Mn	HT*
	Training R^2	Test R^2													
RF	0.77	0.70	90.18	9.50	7.26	1	2	4	5	3	6	7	10	9	8
DT	0.73	0.69	95.31	9.76	7.45	1	2	4	7	8	9	3	10	5	6
XGBoost	0.78	0.74	78.05	8.83	7.07	1	5	6	9	2	3	4	10	7	8
ANN	0.75	0.65	108.04	10.39	8.18	1	2	4	7	10	9	3	5	8	6
AdaBoost	0.75	0.71	88.14	9.38	7.04	1	2	4	6	3	5	7	10	9	8
GB	0.74	0.71	88.03	9.38	7.29	1	2	3	6	4	7	5	10	9	8
CatBoost	0.78	0.73	83.78	9.15	7.32	1	2	3	6	5	8	4	10	9	7
Average	0.76	0.70	90.07	9.48	7.38	1.0	2.4	4.0	6.6	5.0	6.7	4.7	9.3	8.0	7.3

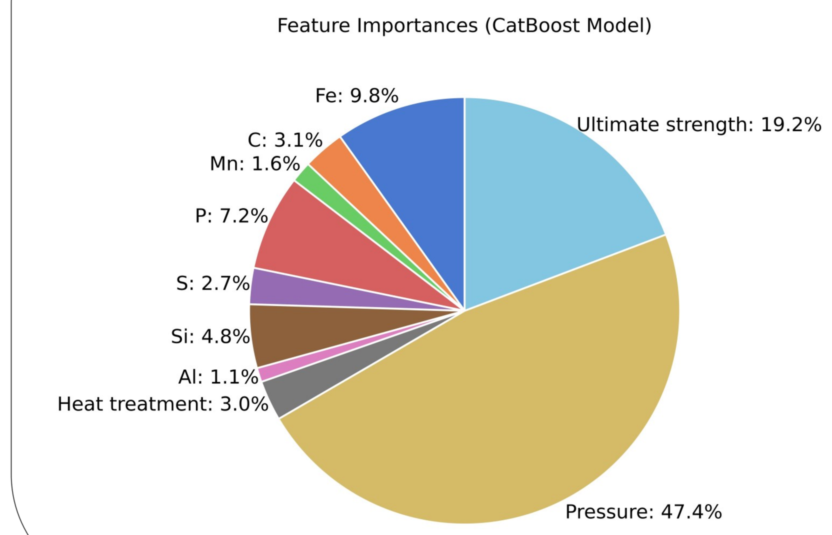
* Heat Treatment

CatBoost Model

Optimum Model's Prediction



Optimum Model's Feature importance



Model Sensitivity Analysis

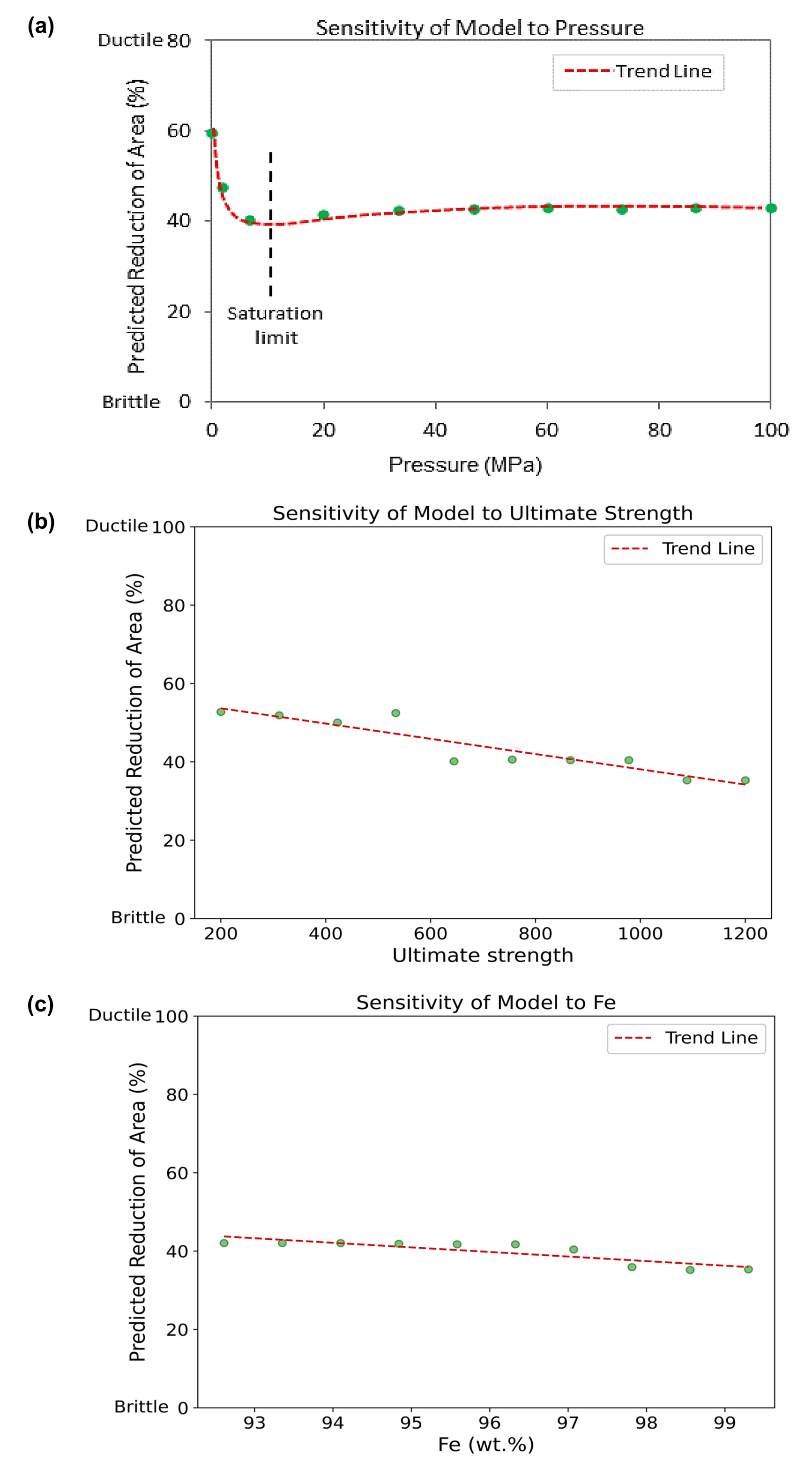


Fig. 6: Sensitivity analysis of pressure (a), ultimate strength (b), and Fe parameters (c) in the CatBoost model

Conclusions

- CatBoost Model predicts hydrogen embrittlement in steel with MAE: 7.32, MSE: 83.78, RMSE: 9.15 (Training R2: 77.62%, Testing R2: 72.50%).
- Top Influencers: Pressure (47.4%) and UTS (19.2%) are critical, with elemental contributions from Iron, Phosphorus, and Silicon.
- Minor Elements: Mn, Al, and S have a combined, yet noteworthy impact.
- Application: Provides insights for material optimization, reducing hydrogen-induced risks.

References

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