ScienceDirect

International Journal of Pressure Vessels and Piping

Volume 210, August 2024, 105247

Guided analysis of fracture toughness and hydrogen-induced embrittlement crack growth rate in quenched-and-tempered steels using machine learning

Sulieman Ibraheem Shelash Al-Hawary [a], Arif Sari [b], Shavan Askar [c], Harikumar Pallathadka [d], Renas Rajab Asaad [e], M.K. Sharma [f]

Show more

Share Cite

https://doi.org/10.1016/j.ijpvp.2024.105247

Get rights and content

Highlights

- Developed ML model predicts fracture toughness and crack growth rate.
- Superior accuracy shown with RMSE: 0.052 for KIC, 0.084 for CGR.
- Input parameter weight factors differ for each output prediction.
- ML enables hydrogen embrittlement identification and characterization.

Abstract

This study focuses on developing a machine learning (ML) model, specifically a Bayesian-optimized deep neural network, leveraging numerical simulation data for the prediction of fracture toughness (K_{IC}) and crack growth rate (CGR) in Quenched-and-Tempered Steel (AISI 4140 alloy) under hydrogen embrittlement conditions. The proposed model demonstrated superior accuracy with Root Mean Squared Error (RMSE) values of 0.052 for K_{IC} and 0.084 for CGR, surpassing conventional ML models including random forest (0.094 for K_{IC}, 0.139 for CGR), gradient boosting (0.184 for K_{IC}, 0.196 for CGR), support vector regression (0.142 for K_{IC}, 0.110 for CGR), and decision tree regression (0.119 for K_{IC}, 0.133 for CGR). The findings also revealed that input parameters such as temperature, hydrogen concentration, and hydrostatic stress carry higher weight factors compared to other parameters in predicting K_{IC}. Similarly, the prediction of high CGR values, ranging from 5.9×10^{-5} to 9.5×10^{-5} m/s, was associated with the importance of hydrostatic stress, strain rate, and initial crack length in the prediction model. This underscores the model's ability to capture the intricate dependencies of output objectives on input features. Furthermore, a comprehensive case study, informed by the ML model, highlights the potential for tuning specific processing input parameters to manage hydrogen embrittlement effectively, contributing to a deeper understanding of its dynamics.

Introduction

Hydrogen embrittlement presents significant challenges in engineering, particularly in materials such as steels, due to its profound detrimental effects [[1], [2], [3]]. It involves the infiltration of hydrogen atoms into the steel matrix, leading to localized pressure buildup. This internal pressure becomes a catalyst for crack initiation and propagation, making the material extremely vulnerable to brittle fracture [[4], [5], [6]]. Consequently, it significantly diminishes the material's capacity to absorb energy through plastic deformation, even under relatively low stress levels. This phenomenon is of utmost importance in pressure vessels and piping applications, where material integrity and reliability are crucial considerations [[7], [8], [9]].

In recent years, extensive research efforts, combining both experimental and numerical approaches, have been undertaken to unravel various facets of hydrogen embrittlement [10,11]. These investigations have delved into understanding the intricate mechanisms, the degradation of material sensitivity, the influence of environmental factors, and more [[12], [13], [14]]. In addition to conventional numerical and experimental techniques, the realm of hydrogen embrittlement characterization has witnessed recent advancements with the emergence of machine learning (ML) approaches [[15], [16], [17]]. These innovative methodologies have been developed to effectively assess and understand hydrogen embrittlement across various alloy types.

For instance, Kim et al. [18] introduced a pioneering ML approach, focusing on predicting hydrogen embrittlement in austenitic steels with a particular emphasis on alloying elements and test conditions, which unveiled the significant influence of Ni and Mo on the embrittlement index. Another approach combined hydrogen thermal desorption spectroscopy (TDS) with ML, creating a regression artificial neural network (ANN) model to predict hydrogen-induced mechanical property degradation in steels [19]. The study demonstrated a strong correlation between TDS data and steel properties, enhancing predictive accuracy. Zhang et al. harnessed machine learning to develop a Fe–H force field for probing hydrogen embrittlement through molecular dynamics simulations [20]. Their findings reveal that elevated hydrogen concentrations ahead of a crack tip accelerate crack propagation, with the degree of acceleration varying based on the type of grain boundary. Meng et al. [21] developed a neural network interatomic potential to probe hydrogen embrittlement at the atomic scale, training it with a comprehensive reference database from density functional theory (DFT) calculations. This model adeptly managed the complex aspects of hydrogen behavior, trapping, and desorption in α-iron, delivering quantitative DFT-level accuracy. In their study, Feng et al. [22] explored the influence of hydrogen embrittlement on various mechanical properties of 316 Stainless Steel, including ductility, tensile strength, and fatigue lifetime, using the MLP-Regressor model to predict S–N curves with and without hydrogen charging. In another work, Phan et al. [23] presented an innovative approach that combined molecular models and Random Forest Regression to predict burst pressure in the context of hydrogen embrittlement. The proposed method not only addressed model uncertainty but also established connections between dimensionless influence functions for both elastic and plastic components of fracture toughness.

While ML approaches have demonstrated remarkable potential in understanding and predicting hydrogen embrittlement, existing research primarily relies on data from experiments and atomic-scale simulations. These methods, however, can be limited in scope and computational cost. Numerical simulations, on the other hand, offer a powerful

tool for investigating complex phenomena at various scales but have seen limited application in generating data for ML models within the context of hydrogen embrittlement [[24], [25], [26], [27], [28]]. This research addresses this gap by establishing a novel framework that integrates comprehensive numerical simulations of fracture toughness with machine learning. This combined approach focuses on quenched-and-tempered steels, specifically AISI 4140, under hydrogen embrittlement conditions. By leveraging the strengths of both numerical simulations and Machine Learning, we aim to achieve a deeper understanding of the mechanisms governing hydrogen embrittlement in this critical material. Numerical simulations can provide detailed data on material properties and hydrogen diffusion, while ML can analyze vast amounts of data to identify complex patterns and relationships. This combined approach will not only contribute to the fundamental understanding of hydrogen's influence on material properties but also pave the way for the development of robust and efficient predictive models. The designed model will enable the prediction of how environmental parameters influence the toughness and degradation of quenched-and-tempered steel. This capability will facilitate the design of real-world structures with greater confidence and minimize the need for trial-and-error approaches.

Section snippets

Computational method

In this section, an ML-based model is presented, capable of predicting the fracture toughness (K_{IC}) and crack growth rate (CGR) in AISI 4140 alloy under hydrogen embrittlement conditions. For this purpose, a comprehensive dataset was first collected for the training process. Hydrogen embrittlement was examined through numerical simulations conducted under various conditions and parameters, thereby creating a robust data space for ML modeling. Detailed methodologies and parameters for the…

Validation of BDNN model

The significance of incorporating regression analysis and comparing it with conventional ML models as the initial steps in validating our ML model lies in their role as benchmarks. Regression analysis provides a fundamental baseline for understanding the relationship between numerical-calculated and ML-predicted results. By contrasting regression results with the performance of conventional ML models, it is also established a solid foundation for assessing the predictive capabilities of our ML…

- Conclusion

In this study, we introduced an ML model, specifically a Bayesian-optimized deep neural network, empowered by numerical simulation data, to predict K_{IC} and CGR in AISI 4140 alloy under hydrogen embrittlement. The main results are as follows.

1) The key outcomes highlight the model's robust predictive performance, as evidenced by high R^2 values of 0.945 for K_{IC} and 0.913 for CGR, coupled with low RMSE values of 0.052 and 0.084, respectively.…

2) The investigation unveiled significant relationships…

…

CRediT authorship contribution statement

Sulieman Ibraheem Shelash Al-Hawary: Writing – review & editing, Writing – original draft, Formal analysis, Data curation, Conceptualization. **Arif Sari:** Writing – review & editing, Writing – original draft, Formal analysis, Conceptualization. **Shavan Askar:** Validation, Methodology, Investigation. **Harikumar Pallathadka:** Validation, Supervision, Software, Investigation. **Renas Rajab Asaad:** Writing – original draft, Validation, Methodology, Investigation. **M.K. Sharma:** Writing – original draft,…

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.…

Recommended articles

References (58)

H. Yang *et al.*
Effects of defect on the hydrogen embrittlement behavior of X80 pipeline steel in hydrogen-blended natural gas environments
Int. J. Hydrogen Energy (2024)

U.S. Meda *et al.*

Challenges associated with hydrogen storage systems due to the hydrogen embrittlement of high strength steels
Int. J. Hydrogen Energy (2023)

M. Röthig *et al.*
A review of gas phase inhibition of gaseous hydrogen embrittlement in pipeline steels
Int. J. Hydrogen Energy (2024)

P. Cavaliere *et al.*
Modelling of the hydrogen embrittlement in austenitic stainless steels
Materialia (2023)

X. Xu *et al.*
Experimental study on the temperature dependence of gaseous hydrogen permeation and hydrogen embrittlement susceptibility of X52 pipeline steel
Eng. Fail. Anal. (2024)

J. Cao
Effect of hydrogen embrittlement on the safety assessment of low-strength hydrogen transmission pipeline
Eng. Fail. Anal. (2024)

P. Cavaliere *et al.*
Modelling of hydrogen diffusion leading to embrittlement in austenitic stainless steels
Int. J. Pres. Ves. Pip. (2024)

S. Peng *et al.*
Influence of hydrogen volume/specimen surface area ratio on hydrogen embrittlement sensitivity of X52 pipeline steel
Int. J. Pres. Ves. Pip. (2024)

S.K. Saha *et al.*
Enhancing the hydrogen embrittlement resistance of medium-carbon high-strength steel by optimizing the tempering temperature
Mater. Char. (2024)

Z. Si *et al.*

An adaptive phase-field simulation for hydrogen embrittlement fracture with multi-patch isogeometric method

Comput. Methods Appl. Mech. Eng. (2024)

View more references

Cited by (0)

View full text