# Predicting fatigue crack growth rate of austenitic stainless steels in water reactors using machine learning algorithms

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***Keywords :*** machine learning, corrosion fatigue crack growth, austenitic stainless steels

## 1. Introduction

Operating history of LWRs has revealed that fatigue was responsible for some cracking incidents in piping, valves, and nozzles used in the reactors, which are made of austenitic stainless steels (SSs) [1]. Accurately predicting the corrosion fatigue (CF) crack growth rate of austenitic stainless SSs is crucial to ensure safe plant. This study proposes a machine learning (ML) approach for such a purpose, as an alternative to the existing empirical models [2-4].

## 2. Methods and Results

### *2.1 Data preparation and preprocessing*

We have collected 806 data on the CF crack growth rates of austenitic SSs in PWR and HWC-BWR water environments from various sources [2-4]. These data were obtained from fracture mechanics tests on Types 304, 316, 304L, and 316L wrought SSs and their respective weld metals. The input features include 11 element contents (Ni, Cr, Mo, C, Mn, Si, N, P, S, Co, and Cu), 3 material properties ($\sigma_{YS}$, $\sigma_u$ and RA), 2 environmental parameters (DH and T), and 3 loading parameters ($\Delta K$, $R$, and $t_r$).

Data preprocessing included feature selection, data splitting, missing value imputation, and data scaling. Feature selection was performed to remove features with excessive number of missing values (e.g., > 50%). Considering this, features Cu, Co, N, and %RA were removed. The dataset was then split into two subsets, i.e., the training (75%) and hold-out test sets (25%). Missing value imputation was performed using the average value of each variable. The features were standardized based on their mean and standard deviation in the training set. The logarithmic scaling was used to transform the crack growth rate values. In the end, 15 features were considered for this analysis.

### *2.2 ML algorithms*

Some of the most widely used algorithms, including gradient boosting (GB), extreme gradient boosting (XGB), categorical boosting (CB). GB [5] implements the boosting technique, which builds decision trees (DTs) sequentially and each newly built DT tries to correct the previous ones. XGB and CB are variants of GB. XGB uses more enhanced regularization techniques to combat overfitting and parallelization during the splitting events in a DT to accelerate the training speed [6]. CB implements an alternative boosting algorithm called ordered boosting and a specific procedure to process categorical features efficiently [7]

### *2.3 Evaluation metrics*

Several evaluation metrics were used to measure the prediction accuracies of ML models. These metrics include mean absolute error (MAE), mean squared error (MSE), and coefficient of determination ($R^2$). MAE, MSE, and R2 are respectively given as:

$$\mathrm{MAE} = \frac{1}{n}\sum_{i=1}^{n}|x_i - y_i| \quad (1)$$

$$\mathrm{MSE} = \frac{1}{n}\sum_{i=1}^{n}(x_i - y_i)^2 \quad (2)$$

$$\mathrm{R}^2 = 1 - \frac{\sum_{i=1}^{n}(x_i - y_i)^2}{\sum_{i=1}^{n}(\bar{y} - y_i)^2} \quad (3)$$

where $x_i$ and $y_i$ denote the i-th predicted and actual output values, respectively.

### *2.4 Hyperparameter tuning*

Two key hyperparameters of each algorithm were first tuned using the grid search method combined with 10-fold cross-validation. These include number of DTs (ND) and maximum tree depth (TD). MSE was used as evaluation metric in the cross-validation. The candidate spaces, default and selected values of hyperparameters for each algorithm are listed in Table 1. It is worth mentioning that most selected values are different from the default ones, confirming the necessity of hyperparameter tuning.

### *2.5 Evaluation of trained ML models*

ML algorithms with their best hyperparameter values were trained using the training set. The trained ML models were then evaluated on the hold-out test set. This step was the final model evaluation to determine

the best suited ML model to predict the CF crack growth rate in austenitic SSs.

Table I: Default and selected hyperparameter values for ML algorithms

| Model | Default value | Selected value |
|---|---|---|
| GB | ND = 100<br>TD = 3 | ND = 200<br>TD =5 |
| XGB | ND = 100<br>TD =6 | ND = 50<br>TD = 5 |
| CB | ND = 1000<br>TD = 6 | ND = 2250<br>TD = 6 |

Table II: Evaluation metrics for ML and empirical models

| Model | MAE | MSE | $R^2$ |
|---|---|---|---|
| GB | 0.102 | 0.024 | 0.963 |
| XGB | 0.109 | 0.033 | 0.95 |
| CB | 0.09 | 0.019 | 0.971 |
| Empirical model [4] | 0.206 | 0.077 | 0.883 |

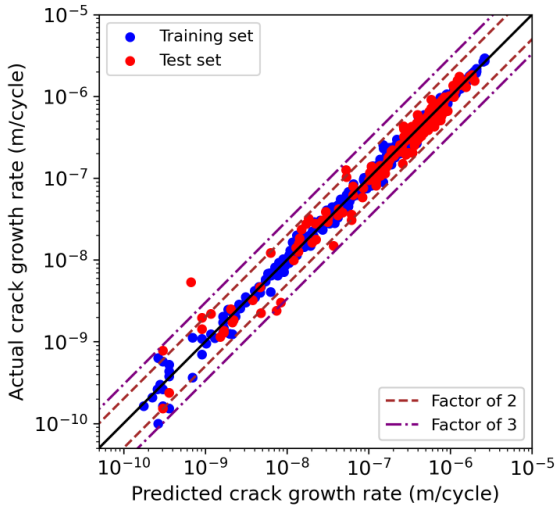


Fig. 1. Parity plot of the CB model.

Table 2 compares the evaluation metrics for the tested ML models computed on the hold-out test set. It was shown that all trained ML models predicted the CF crack growth rate in austenitic SSs exceptionally well. As a comparison, ana empirical model by Baron et al. [4] was also evaluated. The ML models clearly performed better than the empirical model. Among ML models, the CB model performed the best. Figure 1 shows the parity plots for the CB model comparing the predicted and actual CF crack growth rates in the training and hold-out test sets. The model appeared predict both seen and unseen data almost equally well, indicating that overfitting did not occur.

## 3. Conclusions

Some commonly used supervised ML algorithms (GB, XGB, CB) were considered to find the best suited one for the purpose of the current study. Each of them has been shown to perform reasonably well. Among the trained ML models, CB model, trained with an innovative and advanced algorithm, has been shown to outperform the other models. The results of the current study demonstrated that the more accurate prediction for the CF crack growth rate of austenitic SSs can be attained through the implementation of ML techniques.

## REFERENCES

[1] Seifert HP, Ritter S. Environmentally-assisted cracking in austenitic light water reactor structural materials–final report of the KORA-I Project, PSI Report No. 09–03. Paul Scherrer Institute. Villigen PSI. Switzerland. 2009.
[2] Nomura Y, Tsutsumi K, Kanasaki H, Chigusa N, Jokati K, Shimizu H, Hirose T, Ohata H. Fatigue crack growth curve for austenitic stainless steels in PWR environment. Pres Ves Pip 2004;480:63–70.
[3] Cipolla RC, Bamford WH, Hojo K, Nomura Y. Technical Basis for Revision of Code Case N-809 on Reference Fatigue Crack Growth Curves for Austenitic Stainless Steels in Pressurized Water Reactor Environments. In Pressure Vessels and Piping Conference (Vol. 85314 p. V001T01A001); 2021.
[4] Barron KC and Paraventi DJ. A Fatigue Crack Growth Model for Type 304 Austenitic Stainless Steels In a Pressurized Water Reactor Environment. In Pressure Vessels and Piping Conference (Vol. 85314 p. V001T01A015); 2021.
[5] Hastie T, Tibshirani R, Friedman J, Hastie T, Tibshirani R, Friedman J. Boosting and additive trees. The elements of statistical learning: data mining, inference, and prediction 2009:337-387.
[6] Chen T, Guestrin C. August. Xgboost: A scalable tree boosting system. In Proceedings of the 22nd acm sigkdd international conference on knowledge discovery and data mining (pp. 785-794); 2016.
[7] Prokhorenkova L, Gusev G, Vorobev A, Dorogush AV, Gulin A. CatBoost: unbiased boosting with categorical features. Adv Neural Inf Process Syst 2018: 6638–48.