Application of an Artificial Neural Network to Develop Fracture Toughness Predictor of Ferritic Steels Based on Tensile Test Results

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Abstract: Analyzing the fracture toughness of ferritic steels subjected to large temperature variations requires the collection of the fracture toughness (\(K_{\text{IC}}\)) of ferritic steels in the ductile-to-brittle transition region. Consequently, predicting \(K_{\text{IC}}\) from minimal testing has been of interest for a long time. In this study, a Windows-ready \(K_{\text{IC}}\) predictor based on tensile properties (specifically, yield stress \(\sigma_{\text{YSRT}}\) and tensile strength \(\sigma_{\text{BRT}}\) at room temperature (RT) and \(\sigma_{\text{YS}}\) at \(K_{\text{IC}}\) prediction temperature) was developed by applying an artificial neural network (ANN) to 531 \(K_{\text{IC}}\) data points. If the \(\sigma_{\text{YS}}\) temperature dependence can be adequately described using the Zerilli-Armstrong \(\sigma_{\text{YS}}\) master curve (MC), the necessary data for \(K_{\text{IC}}\) prediction are reduced to \(\sigma_{\text{YSRT}}\) and \(\sigma_{\text{BRT}}\). The developed \(K_{\text{IC}}\) predictor successfully predicted \(K_{\text{IC}}\) under arbitrary conditions. Compared with the existing ASTM E1921 \(K_{\text{IC}}\) MC, the developed \(K_{\text{IC}}\) predictor was especially effective in cases where \(\sigma_{\text{B}}/\sigma_{\text{YS}}\) of the material was larger than that of RPV steel.

Keywords: fracture toughness; machine learning; artificial neural network; predictor; yield stress; tensile strength; specimen size

1. Introduction

Both researchers and practitioners have characterized the fracture toughness (\(K_{\text{IC}}\)) of ferritic steels in the ductile-to-brittle transition (DBT) region, which is key for analyzing the structural integrity of cracked structures subjected to large temperature changes. \(K_{\text{IC}}\) is associated with (I) a large temperature dependence (a change of approximately 400% corresponding to a temperature change of 100 °C) [1–10]; (II) specimen-thickness dependence (roughly, \(K_{\text{IC}} \propto 1/(\text{specimen thickness})^{1/4}\)) [8,11–21]; and (III) large scatter (approximately ±100% variation around the median value) [8,22,23]. Thus, understanding these three effects is necessary for efficient \(K_{\text{IC}}\) data collection.

Since Ritchie and Knott introduced the idea of using critical stress and distance to predict fracture toughness temperature dependence [4], researchers who explicitly or implicitly applied this idea have obtained results that demonstrate a strong correlation between the temperature dependence of fracture toughness and that of yield stress (\(\sigma_{\text{YS}}\)) [5,6]. Wallin observed that the increase in fracture toughness with increasing temperature is not sensitive to steel alloying, heat treatment, or irradiation [7]. This observation led to the concept of a universal curve shape that applies to all ferritic steels, i.e., the difference in materials is reflected by the temperature shift. This concept is now known as the master curve (MC) method, as described by the American Society for Testing and Materials (ASTM) E1921 [8]. The existence of a \(K_{\text{IC}}\) MC was physically supported by Kirk et al. based on dislocation mechanics considerations [9,10]. They argued that the temperature dependence of \(K_{\text{IC}}\) is related to the temperature dependence of the strain energy density (SED). Furthermore,
because all steels with body-centered cubic (BCC) lattice structures exhibit a unified $\sigma_{YS}$ temperature dependence, as described by the Zerilli–Armstrong (Z–A) constitutive model (i.e., Z–A $\sigma_{YS}$ MC) [24], the existence of a BCC iron lattice structure is the sole factor needed to ensure that $K_{JC}$ in the DBT region has an MC. Note that Kirk et al. implicitly assumed that the tensile-to-yield stress ratio does not vary with materials, which is not true, and will be a source of deviation from the MC. For example, the failure of this MC to evaluate increases in $K_{JC}$ at high temperatures has been reported for non-reactor pressure vessel (RPV) steels [25,26]. Despite the successful application of $K_{JC}$ MC to RPV steels, a reexamination of the basis of $K_{JC}$ MC existence and additional application limits must be reexamined for the application of ASTM E1921 MC to ferritic steels in general and not be limited to RPV steels.

The size dependence of $K_{JC}$ has been understood based on the weakest link theory deduced as $K_{JC} \propto 1/(\text{specimen thickness})^{1/4}$ [17], but because this relationship cannot describe the existence of a lower-bound $K_{JC}$ for large specimens, researchers have begun to investigate the size dependence of $K_{JC}$ as the critical stress distribution ahead of a crack-tip requires a second parameter in addition to $J$ (J–A, J–T approach, etc.) [18,19], which is categorized as a crack-tip constraint issue. Consequently, it appears that the development of a deterministic and data-driven size effect formula is possible. ASTM E1921 provides a semi-empirical size effect formula based on the $K_{JC}$ of a 1-inch-thick specimen, which considers a lower-bound $K_{JC}$ of 20 MPa·m$^{1/2}$ and proportionality to $1/(\text{specimen thickness})^{1/4}$. There are various opinions regarding this lower-bound value [27–30]; thus, the establishment of a data-driven size effect formula that does not depend on the $\propto 1/(\text{specimen thickness})^{1/4}$ relationship seems possible and necessary.

The statistical nature of fracture toughness has been modeled using the Weibull distribution; some researchers used stress [22] and some used $K_{JC}$ [8] as the model mean parameter. The idea of using Weibull distributions stems from the understanding that the cleavage fracture can be modeled using the weakest link theory. ASTM E1921 [8] applies a three-parameter Weibull distribution, which assumes a shape parameter of four and a position parameter of $20 \text{ MPa} \cdot \text{m}^{1/2}$. The failure of this model to predict the scatter in $K_{JC}$ has also been reported; Weibull parameters (shape and position) vary as functions of the specimen size and temperature, and the parameters differ from those specified in ASTM E1921 [31,32]. If the observed model parameters differ from the assumed parameters, the predicted $K_{JC}$ and scatter deviate from the measured values. Hence, a more practical method that can potentially prevent the mismatch of the assumed statistical model, i.e., a data-driven approach, is necessary.

Considering the three aforementioned issues, it was considered that a data-driven $K_{JC}$ predictor that captured features of a variety of BCC metals could improve $K_{JC}$ prediction accuracy. Another idea was to replace time- and material-consuming fracture toughness tests with tensile tests, assuming that $K_{JC}$ has a direct relationship with SED obtained via tensile tests. Thus, the artificial neural network (ANN) approach was applied to 531 $K_{JC}$ data collected in our previous works [30,33] to construct a $K_{JC}$ predictor based on tensile test properties, thereby eliminating the need to conduct fracture toughness tests. The data were obtained for five heats of RPV and seven heats of non-RPV steels. The widths $W$ of the specimens ranged from 20 to 203.2 mm, and the thickness-to-width ratio $B/W$ was limited to 0.5 (i.e., data obtained with PCCV specimens of $B/W = 1$ were excluded). As a result, a Windows-ready $K_{JC}$ predictor, which enables $K_{JC}$ prediction by giving specimen size, tensile and yield stress, was developed. Time- and material-consuming fracture toughness tests are no more necessary.

2. Materials and Methods

2.1. Selection of Machine Learning Model

Machine learning models are used in many fields, such as search engines, image classification, and voice recognition, and various methods have been proposed according to the application. In this study, a tool to predict the fracture toughness $K_{JC}$ of a material
under arbitrary conditions such as the specimen size and temperature, without performing the fracture toughness test, was conducted; this is treated as a regression issue. There are various algorithms for machine learning models for regression. In this study, a multilayer perceptron (MLP) was classified into an ANN that can express complex nonlinear relationships. The regression model was constructed using the MLP regressor, which is a scikit-learn library of the general-purpose programming language Python [34].

2.2. Overview of Multilayer Perceptron in an Artificial Neural Network

Figure 1 shows a schematic diagram of the MLP network. The MLP is a hierarchical network comprising an input layer, a hidden layer, and an output layer; the unit of the hidden layer is completely connected to the input and output layers [34,35].

In Figure 1, only one hidden layer is schematically shown; however, in general, multiple hidden layers are used to enhance the expressiveness of the model. The unit in the hidden layer (hereinafter, referred to as the activation unit) and the number of hidden layers are parameters that were adjusted according to the application. In this study, a tool to predict the fracture toughness of a material under arbitrary conditions such as the specimen size and temperature, without performing the fracture toughness test, was conducted; this is treated as a regression issue. There are various algorithms for machine learning models for regression. In this study, a multilayer perceptron (MLP) was classified into an ANN that can express complex nonlinear relationships. The regression model was constructed using the MLP regressor, which is a scikit-learn library of the general-purpose programming language Python [34].

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![Figure 1. Schematic diagram of multilayer perceptron in an ANN.](image)

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Here, $w_{hi}$ is the connection weight, $X_0$ is a constant called bias, and $\phi$ of Equation (1) is a function called the activation function. For the activation function, a function with differentiable nonlinearity was selected to enhance the expressiveness of the model. In this study, the rectified linear unit (ReLU) function $\phi(z) = \max(0, z)$ was used and $a_j$ was assigned to the hidden layer. The total number $k$ of $a_j$ (the number of nodes in the hidden layer) and the number of hidden layers are parameters that were adjusted according to the learning accuracy. The output value $f(X)$ can be obtained via Equation (2).

$$a_j = \phi \left( \sum_{i=0}^{n} w_{hi} X_i \right)$$  \hspace{1cm} (1)

$$f(X) = \phi \left( \sum_{j=0}^{k} w_{oj} a_j \right),$$  \hspace{1cm} (2)

where $w_{oj}$ denotes the connection weight. In Equations (1) and (2), the connection weights $w_{hi}, w_{oj}$ are unknown constants and can be obtained from the combination of known input and output values. By assuming that the known teaching data (true value) are $Y$.
(to distinguish it from \( f(X) \), predicted from the input value \( X_i \) from Equation (2)), the connection weights can be updated in Equation (3), using the loss function \( E \).

\[
E = \frac{1}{2} \sum_l (Y_l - f_l(X))^2 + \frac{\alpha}{2} \sum_l |w_l|^2
\]  

(3)

Here, the first term in Equation (3) is the sum of the squared residuals of the teaching data \( Y \) and the output value \( f(X) \), and the second term is a regularization term using the \( L^2 \) norm to suppress overfitting. \( \alpha \) is a parameter that is adjusted according to learning accuracy. Overfitting is a problem in which training data are overfitted and unknown data cannot be effectively generalized. Several effective optimization algorithms have been developed to avoid falling into a locally optimal solution for updating the connection weights. In this study, adaptive moment estimation (Adam) \[36\] was used. The connection weight \( w \) is updated using Equations (4)–(9).

\[
W^{(t)} = w^{(t-1)} - \eta \frac{m^{(t)}}{\sqrt{v^{(t)}} + \epsilon}
\]  

(4)

\[
m^{(t)} = \frac{m^{(t)}}{1 - \beta^1}
\]  

(5)

\[
v^{(t)} = \frac{v^{(t)}}{1 - \beta^2}
\]  

(6)

\[
m^{(t)} = \beta_1 m^{(t-1)} + (1 - \beta_1) \frac{\partial E}{\partial w}
\]  

(7)

\[
v^{(t)} = \beta_2 v^{(t-1)} + (1 - \beta_2) \left( \frac{\partial E}{\partial w} \right)^2
\]  

(8)

\[
m^{(0)} = v^{(0)} = 0
\]  

(9)

The recommended values were used for the adjustment parameters \( \eta, \beta_1, \beta_2, \) and \( \epsilon \) \[36\]. The error backpropagation method to update the connection weight was used, which calculates the gradient of the loss function by moving backward from the output layer. This method is known to be less computationally expensive than updating weights in the forward direction \[37\].

2.3. Goodness Valuation of Constructed Learning Model

The goodness of valuation of the constructed machine learning model is based on the coefficient of determination \( R^2 \) in Equation (10), where \( n \) is the amount of teaching data, \( Y_i \) is the true objective value, \( f(X) \) is the predicted objective value, and the average value of the true objective values is \( \sigma_Y \).

\[
R^2 = 1 - \frac{\sum_i (Y_i - f_i(X))^2}{\sum_i (Y_i - \mu_Y)^2}
\]  

(10)

The coefficient of determination indicates the goodness of fit of the regression model and is an evaluation index for assessing how well the predicted and true values match. \( R^2 = 1 \) when the true and predicted values are the same. There is no clear standard for the coefficient of determination, but it can be considered compatible if it is approximately 0.5 or more.
2.4. Dataset

For machine learning, the fracture toughness test data of 531 ferritic steels in the DBTT region obtained by the authors or previous studies were used. Table 1 presents the chemical compositions of the test specimens of the materials considered in the teaching data.

| Heat No. | Material               | C      | Si    | Mn    | P      | S      | Ni    | Cr    | Mo    | V      | Cu    | Nb    | Ti    | Al    |
|----------|------------------------|--------|-------|-------|--------|--------|-------|-------|-------|--------|-------|-------|-------|-------|
| 1        | MiuraSFVQ1A [38]       | 0.18   | 0.18  | 1.46  | 0.002  | <0.001 | 0.90  | 0.12  | 0.52  | <0.01  | -     | -     | -     | -     |
| 2        | Gopalan20MnMoNi55 [39] | 0.20   | 0.24  | 1.38  | 0.011  | 0.005  | 0.52  | 0.06  | 0.30  | -      | 0.032 | -     | 0.068 | -     |
| 3        | ShorehamA533B [40]     | 0.21   | 0.24  | 1.23  | 0.004  | 0.008  | 0.63  | 0.09  | 0.53  | -      | 0.08  | -     | 0.04  | -     |
| 4        | MiuraSQV2Ah1 [38]     | 0.22   | 0.25  | 1.44  | 0.002  | 0.008  | 0.69  | 0.11  | 0.57  | -      | -     | -     | -     | -     |
| 5        | MiuraSQV2Ah2 [38]     | 0.22   | 0.25  | 1.46  | 0.002  | 0.008  | 0.69  | 0.11  | 0.57  | -      | -     | -     | -     | -     |
| 6        | GarciaS275JR [41]      | 0.18   | 0.26  | 1.18  | 0.012  | 0.009  | <0.085| <0.018| <0.12 | <0.02  | 0.032 | -     | -     | -     |
| 7        | GarciaS355J2 [41]     | 0.2    | 0.31  | 1.39  | <0.012 | 0.008  | 0.09  | 0.05  | <0.12 | 0.02   | 0.06  | -     | 0.022 | 0.014 |
| 8        | CiceroS460M [42]      | 0.12   | 0.45  | 1.49  | 0.012  | 0.001  | 0.016 | 0.062 | -     | 0.066  | 0.011 | 0.036 | 0.003 | 0.048 |
| 9        | CiceroS690Q [42]      | 0.15   | 0.40  | 1.42  | 0.006  | 0.001  | 0.160 | 0.020 | -     | 0.058  | 0.010 | 0.029 | 0.003 | 0.056 |
| 10       | MeshiiFY2017SCM440 [25]| 0.39   | 0.17  | 0.62  | 0.011  | 0.002  | 0.07  | 0.02  | 0.17  | -      | 0.10  | -     | -     | -     |
| 11       | MeshiiFY2012SS5C [6]   | 0.55   | 0.17  | 0.61  | 0.015  | 0.004  | 0.07  | 0.08  | -     | -      | 0.13  | -     | -     | -     |
| 12       | MeshiiFY2016SS5C [26]  | 0.54   | 0.17  | 0.61  | 0.014  | 0.003  | 0.06  | 0.12  | -     | -      | -     | -     | -     | -     |

Tables 2–4 summarize the material heats (heat No. 1–12) used in this study, nt indicates the specimen thickness, and n is expressed in multiples of 25 mm. They are fundamentally extracted from previous work [30,33], but differ slightly in terms of the following: (1) $K_{JC} > K_{JC(ulimit)}$ invalid data were excluded, (2) $K_{JC}$ data were limited to cases obtained with standard specimens of thickness-to-width ratio $B/W = 0.5$, (3) When there were no $\sigma_{YS}$ data for the fracture toughness test temperature, it was obtained by using the following modified Z–A $\sigma_{YS}$ temperature-dependent MC [9]

$$
\sigma_{0ZA}(T) = \sigma_{0RT} + C_1 \exp\left[\left(\frac{T + 273.15}{C_3 + C_4 \log(\dot{\varepsilon})}\right) - 49.6\right] (MPa),
$$

where $T$ is the temperature (°C), $C_1 = 1033$ (MPa), $C_3 = 0.00698$ (1/K), $C_4 = 0.000415$ (1/K), and $\dot{\varepsilon} = 0.0004$ (1/s). The three Miura heats (heat No. 1, 4, 5) were another exception for which linear interpolation of raw data was used because the fracture toughness and tensile test temperatures were different.

| Heat No. | Material               | Specimen Type | Temps. (°C) | Num. of Temp. | $\sigma_{YS}$ (MPa) | $\sigma_{YSRT}$ (MPa) | $\sigma_{BRT}$ (MPa) | Num. of Specimens | $T_0$ (°C) |
|----------|------------------------|---------------|-------------|---------------|---------------------|----------------------|-------------------|-----------------|------------|
| 1        | MiuraSFVQ1A [38]      | 1TC(T)        | −120−−60    | 4             | 530−640            | 454                  | 594               | 32              | −98       |
|          |                        | 2TC(T)        | −120−−60    | 4             | 530−640            | 454                  | 594               | 16              | −98       |
|          |                        | 4TC(T)        | −100−−80    | 2             | 560−607            | 454                  | 594               | 12              | −98       |
|          |                        | 0.4TC(T)      | −140−−80    | 4             | 560−695            | 454                  | 594               | 34              | −98       |
|          |                        | 0.4TSE(B)     | −140−−80    | 4             | 560−695            | 454                  | 594               | 29              | −98       |
| 2        | Gopalan20MnMoNi55 [39] | 1TC(T)        | −140−−80    | 3             | 560−667            | 479                  | 616               | 18              | −133      |
|          |                        | 0.5TC(T)      | −140−−80    | 3             | 560−667            | 479                  | 616               | 12              | −133      |
Table 3. $K_{jc}$ data used to construct the proposed tensile property-based $K_{jc}$ MC: RPV steel ASTM A533B and equivalent.

| Heat No. | Material          | Specimen Type | Temps. (°C) | Num. of Temp. | $\sigma_{YS}$ (MPa) | $\sigma_{YSRT}$ (MPa) | $\sigma_{BRT}$ (MPa) | Num. of Specimens | $T_0$ (°C) |
|---------|------------------|---------------|-------------|---------------|----------------------|-----------------------|---------------------|-------------------|-------------|
| 3       | Shoreham A533B   | 1TC(T)        | −100−−64    | 3             | 355–586              | 488                   | 644                 | 18                | −91         |
| 4       | Miura SQV2Ah1    | 1TC(T)        | −100−−60    | 3             | 544–600              | 473                   | 625                 | 14                | −93         |
|         |                  | 2TC(T)        | −100−−60    | 3             | 544–600              | 473                   | 625                 | 14                | −93         |
|         |                  | 4TC(T)        | −80−−60     | 2             | 544–566              | 473                   | 625                 | 12                | −93         |
|         |                  | 0.4TC(T)      | −120−−60    | 4             | 544–658              | 473                   | 625                 | 32                | −93         |
|         |                  | 0.4TSE(B)     | −120−−60    | 4             | 544–658              | 473                   | 625                 | 29                | −93         |
| 5       | Miura SQV2Ah2    | 1TC(T)        | −140−−80    | 4             | 542–709              | 461                   | 602                 | 23                | −121        |
|         |                  | 2TC(T)        | −100−−80    | 2             | 542–607              | 461                   | 602                 | 12                | −121        |
|         |                  | 4TC(T)        | −100−−80    | 2             | 542–607              | 461                   | 602                 | 12                | −121        |
|         |                  | 0.4TC(T)      | −140−−80    | 4             | 542–709              | 461                   | 602                 | 33                | −121        |
|         |                  | 0.4TSE(B)     | −140−−80    | 4             | 542–709              | 461                   | 602                 | 32                | −121        |

*: Side-grooved specimens.

Table 4. $K_{jc}$ data used to construct the proposed tensile property-based MC: non-RPV steels.

| Heat No. | Material          | Specimen Type | Temps. (°C) | Num. of Temp. | $\sigma_{YS}$ (MPa) | $\sigma_{YSRT}$ (MPa) | $\sigma_{BRT}$ (MPa) | Num. of Specimens | $T_0$ (°C) |
|---------|------------------|---------------|-------------|---------------|----------------------|-----------------------|---------------------|-------------------|-------------|
| 6       | Garcia S275JR    | 1TC(T)        | −50−−10     | 3             | 338−349              | 328                   | 519                 | 14                | −26         |
| 7       | Garcia S355JR    | 1TC(T)        | −150−−100   | 3             | 426−528              | 375                   | 558                 | 13                | −134        |
| 8       | Cicero S460M     | 0.6TSE(B)     | −140−−100   | 3             | 597−686              | 473                   | 595                 | 14                | −92         |
| 9       | Cicero S690Q     | 0.6TSE(B)     | −140−−100   | 3             | 899−988              | 775                   | 832                 | 13                | −111        |
| 10      | Meshii FY2017 SCM440 | 0.9TSE(B) | −55−−100   | 4             | 410−524              | 459                   | 796                 | 18                | 17          |
|         |                  | 0.5TSE(B)     | −55−−100    | 4             | 410−524              | 459                   | 796                 | 22                | 17          |
| 11      | Meshii FY2012 S55C | 0.5TSE(B) | −25−−20    | 3             | 394−444              | 394                   | 707                 | 17                | 27          |
| 12      | Meshii FY2016 S55C | 0.9TSE(B) | −45−−35    | 3             | 375−475              | 382                   | 685                 | 17                | 15          |
|         |                  | 0.5TSE(B)     | −85−−20     | 3             | 382−562              | 382                   | 685                 | 19                | 15          |

The objective variable was $K_{jc}$. Assuming a direct relationship between the SED temperature dependence and that of $K_{jc}$, $\sigma_B$ temperature dependence was the first candidate explanatory parameter. However, considering that (i) $\sigma_B/\sigma_{YS}$ temperature dependence is small, (ii) ferritic steel has a $\sigma_{YS}$ temperature-dependent MC such as Z−A MC, and (iii) $\sigma_B/\sigma_{YS}$ at RT is usually easily available, $\sigma_B$ and $\sigma_{YS}$ at RT, and $\sigma_{YS}$ at $K_{jc}$ test temperatures and specimen width $W$ were selected as the explanatory variables. To optimize the connection weight, 371 points, i.e., 70% of the 531 points in the known dataset, were used as the training data. The data were divided by “train_test_split” of Python’s scikit-learn library. If the digits of the input value and output value to be learned are significantly different, the influence of variables with small digits may not be fully considered in learning. Therefore, in this study, the input values $W, \sigma_{YS}, \sigma_{YSRT}, \sigma_{BRT}$, and output value $K_{jc}$ were standardized, as shown in Equation (12).

$$
\left( \begin{array}{c}
W \text{(mm)} \\
\sigma_{YS} \text{(MPa)} \\
\sigma_{YSRT} \text{(MPa)} \\
\sigma_{BRT} \text{(MPa)} \\
K_{jc} \text{ (MPa·m}^{1/2} \text{)}
\end{array} \right)_{\text{Normalized}} = \left( \begin{array}{c}
W/50 \\
\sigma_{YS}/550 \\
\sigma_{YSRT}/550 \\
\sigma_{BRT}/550 \\
K_{jc}/100
\end{array} \right)
$$

(12)

Here, with reference to ASTM E1921, $W$ was normalized using the width 50 mm of a 1T specimen, and the yield stress and tensile strength were normalized using the average value of 550 MPa of the yield stress of 275 to 825 MPa in the allowable temperature range targeted by the standard. $K_{jc}$ was normalized to a fracture toughness of value 100 MPa·m$^{1/2}$ at the reference temperature.
2.5. Fracture Toughness Prediction by the Constructed Learning Model

Table 5 presents a list of hyperparameters used for the machine learning model in this study. Using the data in Tables 2–4 and the parameters in Table 5, which is currently an invariant model, the coefficient of determination $R^2$ of the developed $K_{Jc}$ predictor was 0.61 for the training data and 0.53 for the test data. Table 6 presents the explanation variables for predicting fracture toughness $K_{Jc}$.

Table 5. Hyperparameters used for the learning model.

| Parameters                      | Value         |
|--------------------------------|---------------|
| Number of hidden layers        | 4             |
| Number of hidden layer nodes   | 100, 50, 25, 10 |
| Activation function            | ReLU          |
| Solver                         | Adam          |
| $\alpha$                       | 0.01          |
| $\eta$                         | 0.001         |
| $\beta_1$                      | 0.9           |
| $\beta_2$                      | 0.999         |
| $\epsilon$                     | $1.0 \times 10^{-8}$ |

Table 6. Explanatory variables for case studies applied to the developed tool.

| Heat No. | Material       | W (mm) | $T$ (°C)   | $\sigma_{YSRT}$ (MPa) | $\sigma_{YS}$ (MPa) | $\sigma_{BRT}$ (MPa) |
|----------|----------------|--------|------------|-----------------------|---------------------|---------------------|
| 1        | Miura SFVQ1A   | 20     | $-140, -120, -100, -80$ | 454                   | 695, 640, 607, 560  | 594                 |
|          |                | 50.8   | $-120, -100, -80, -60$ | 454                   | 640, 607, 560, 530  | 594                 |
|          |                | 101.6  | $-120, -100, -80, -60$ | 454                   | 640, 607, 560, 530  | 594                 |
|          |                | 203.2  | $-80, -100$      | 454                   | 607, 560            | 594                 |
| 10       | MeshiiFY2017SCM440 | 25     | $-55, 20, 60$   | 459                   | 524, 459, 435, 410  | 796                 |
|          |                | 46     | $-55, 20, 60$   | 459                   | 524, 459, 435, 410  | 796                 |

The input data ($W, \sigma_{YS}, \sigma_{YSRT}, \sigma_{BRT}$) for the developed $K_{Jc}$ predictor and output window after its execution (the coefficient of determination $R^2$ and the predicted $K_{Jc}$) are shown in Figure 2. In Figure 3, the comparison of $K_{Jc}$ of ASTM E1921 MC and predicted $K_{Jc}$ by the predictor is shown. In Figure 3, the horizontal axis is $T$, the vertical axis $K_{Jc(1T)}$ is the test data, and the predicted $K_{Jc}$ is converted to 1T thickness. The $K_{Jc}$ of the ASTM E1921 MC is plotted as a black solid line, the $K_{Jc}$ of the test data are plotted as open black symbols, and the predicted conditions listed in Table 6 are plotted as open red symbols. In Figure 3a, for RPV steel, both the $K_{Jc}$ by the ASTM E1921 MC and the predicted $K_{Jc}$ by this model are in agreement with the test results. However, in Figure 3b for SCM440, although the $K_{Jc}$ by the ASTM E1921 MC significantly differs from the test results at high temperatures, the predicted $K_{Jc}$ values by this model are in agreement with the test results.
Adding an axes using the same arguments as a previous axes currently raises the earlier instance. In a future version, a new instance will always be created and returned. Meanwhile, this warning can be suppressed, and the future behavior is ensured, by passing a unique label to each axes instance.

### Figure 3.

![Comparison of Kjc of ASTM E1921 MC (solid line) and predicted Kjc by the predictor (open red symbols): Dataset used for training model and result of predicted Kjc. (a) RPV steel (Miura SFVQ1A); (b) Meshii FY2017SCM440. Kjc predicted by the developed predictor accurately predicted Kjc regardless of materials.](image)

#### 3. Discussion

By applying the ANN, a Kjc predictor for ferritic steels that only requires tensile properties (i.e., σYS at the desired temperature for predicting Kjc, and the RT values σYSRT and σBRT) were derived. This method eliminates the need for time- and material-consuming fracture toughness tests. The tool for predicting Kjc by considering the specimen size and material properties is based on 531 fracture toughness test data values obtained from five RPV steel heats and seven non-RPV steel heats. The specimen sizes ranged from 0.4T to 20T to learn the size effect, the yield stress ranged from 328 to 775, and the tensile strength ranged from 519 to 832 to learn the material properties. The data range used in the training was equal to the application limit of the predictor. The developed Kjc predictor successfully predicted training data with $R^2 = 0.61$ and test data with $R^2 = 0.53$.

To predict Kjc at a specific temperature of interest, the user needs σYS at this temperature as well as σYSRT and σBRT at RT. If the material of interest is known to be well fitted by the Z–A σYS MC, the quantities for which test data are necessary for Kjc prediction are only σYSRT and σBRT.

A considerable advantage of the proposed Kjc predictor is that fracture toughness tests are not necessary to predict Kjc. The key novel idea here is to use tensile properties (such as τYS and σB) and specimen size W.

Although the developed Kjc predictor predicts one Kjc for a combination of explanatory variables, the predicted Kjc fracture probability is predicted by assuming the probability density distribution of the data to be learned (e.g., Weibull distribution). It is also possible to evaluate it together, which is a future issue.

According to Tables 2–4, the $(σ_B/σ_{YS})_{RT}$ of non-RPV and RPV are different. Accepting Kirk’s opinion that Kjc and SED correspond, ASTM E1921 MC may deviate from non-RPV. However, this Kjc predictor has an advantage in that it considers this. On this point, the developed Kjc predictor, compared with the existing ASTM E1921 Kjc MC, is expected to be especially effective in cases where $σ_B/σ_{YS}$ of the material is larger than that of RPV steel.

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**Figure 2. Input data (left figure) and window after execution (right figure).**

(a) (b)

![Input data; Output window.](image)
4. Conclusions

In this study, a tool was developed that can predict $K_{Jc}$ for an arbitrary specimen size $W$ and material properties ($\sigma_{YSRT}$, $\sigma_{YS}$, $\sigma_{BRT}$) via an ANN applied to 531 fracture toughness test data values. Currently, the conditions applicable to the tool are material properties ranging from $\sigma_{YSRT} = 328$ to 775 MPa, $\sigma_{BRT} = 519$ to 832 MPa, specimen size ranging from 0.4T to 4T and its types are CT and SEB. By using the tool developed through the application of data-driven ideas, it is possible to predict the fracture toughness at this temperature from the tensile test results and the specimen size at the target temperature of the fracture toughness without performing a fracture toughness test. In the future, it is planned to predict the predicted probability of fracture toughness.

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Nomenclature

- $B$: test specimen thickness
- $J$: $j$-integral
- $K_{Jc}$: fracture toughness
- $T$: temperature ($^\circ$C)
- $T_0$: ASTM E1921 MC reference temperature ($^\circ$C) for a 25 mm thick specimen with a fracture toughness of 100 MPa·m$^{1/2}$
- $W$: specimen width
- $\sigma_{YS}$, $\sigma_{B}$: yield (0.2% proof) and tensile strength
- $\sigma_{YZA}$: yield stress at the temperature $T$ ($^\circ$C) described by the Zerilli equation (i.e., Equation (11))
- $R^2$: coefficient of determination
- $X_i$: input value of MLP
- $a_j$: activation unit of MLP
- $n$: number of input value
- $k$: number of activation unit
- $f(X)$: output value of MLP
- $w^h_{ij}$: connection weight between input value $X_i$ and activation unit $a_j$
- $\phi$: activation function
- $w^o_{aj}$: connection weight between activation unit $a_j$ and output value $f(X)$
- $Y$: teaching data
- $E$: loss function
- $\alpha$: regularization strength of $L^2$ norm term
- $w^{(t)}$: connection weight at timestep $t$ in Adam
- $m^{(t)}$: exponential moving averages of the gradient at timestep $t$ in Adam
- $v^{(t)}$: exponential moving averages of the squared gradient at timestep $t$ in Adam
- $\hat{m}^{(t)}$: bias-corrected first moment estimates at timestep $t$ in Adam
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$\hat{v}(t)$ bias-corrected second raw moment estimates at timestep $t$ in Adam

$\eta$ learning rate in Adam

$\epsilon$ hyper parameter for numerical stability in Adam

$\beta_1$ hyper parameter for $m(t)$ in Adam

$\beta_2$ hyper parameter for $v(t)$ in Adam

$\mu_Y$ average value of the true objective values

Abbreviations

ASTM American Society for Testing and Materials

BCC body-centered cubic

C(T) compact tension; specimen type

DBT ductile-to-brittle transition

MC master curve

$nT$ notation used to indicate specimen thickness, where $n$ is expressed in multiples of 25 mm

RPV reactor pressure vessel

RT room temperature

SE(B) single-edge notched bend bar; specimen type

Z–A Zerilli–Armstrong

SED strain energy density

PCCV pre-cracked Charpy V-notch; specimen type

MLP multiplayer perceptron

ANN artificial neural network

ReLU rectified linear unit

Adam adaptive moment estimation

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