Mechanical properties prediction of structural stainless steel using Random Forest

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ABSTRACT

It is necessary to clarify the ultimate strength properties of the stainless steel structure to promote structural design rationalization. Rasmussen proposed a prediction equation that accurately expresses the stress-strain curve of stainless steel and can analyze the ultimate strength. The equation requires tensile strength and uniform elongation in addition to the elastic modulus, 0.2% proof stress, and hardening exponent. For this reason, Rasmussen collected existing material test results on stainless steel to establish the prediction equation based on regression analysis, which can estimate tensile strength and uniform elongation. However, there is concern over the accuracy of prediction equations because regression analysis is not always easy to consider non-linearity between explanatory and objective variables. Recent studies have shown that Random Forest, which is one of machine learning-methods, has performed best in predicting material properties from features of the materials. Accordingly, the present study predicted tensile strength and uniform elongation from other parameters by Random Forest. In addition, prediction accuracy of the values using Random Forest compared with that of those using prediction equations. As a result, Random Forest exhibited generally high prediction accuracy compared to prediction equations.

KEY WORDS: structural stainless steel, mechanical properties, random forest

１．Introduction

Minimization of maintenance work, reducing of Life cycle cost (LCC), and prolonging life are required for steel bridges which will be replaced or renewed in the future. The use of structural stainless steel is expected to be able to meet these requirements. From the viewpoint of material properties, austenitic, duplex and ferritic stainless steels are suitable for structural use. Among them, duplex stainless steel has already employed as structural member of the bridge in mainly European countries[1].

Structural design standard is needed to apply stainless steel to structural members of the bridge. Design standard for welded stainless steel structures has been established in Europe[2]. However, the ultimate strength properties of stainless steel structures are needed to be clarified to promote rationalization of the design, because there are not a few design provisions which were based on design standards for structural carbon steel structures.

Unlike common structural carbon steel, stress-strain curve of stainless steel exhibits rounded shape. Therefore, a constitutive equation able to express the stress-strain curve accurately is required for the ultimate strength analysis of stainless steel structures. Several constitutive equations for stainless steel have been proposed in existing studies[3)-5)].

Although Rasmussen[5] proposed a constitutive equation which can express accurately stress-strain curve of stainless steel, elastic modulus E, 0.2% proof stress $\sigma_{0.2}$, hardening exponent n, tensile strength σ_u and uniform elongation ε_u are required for describing the equation. Rasmussen said that it is easy to gain values of E, $\sigma_{0.2}$ and n from design standard whereas values of σ_u and ε_u cannot easily be obtained. For this reason, he collected existing material test results on stainless steel and proposed prediction equations which can estimate σ_u and ε_u from E, $\sigma_{0.2}$ and n, based on regression

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analysis. However, regression analysis is not always easy to consider non-linearity between explanatory and objective variables. Therefore, there is concern over the accuracy of prediction equations.

However, in the data science field, which has become increasingly popular, several prediction methods have been developed to analyze causal relationships between data and to find laws governing the relationship between characteristic values for big data. It is well known that machine learning and deep learning are effective examples of this kind of method.

A number of machine learning-methods have been developed, such as Random Forest (hereafter abbreviated to "RF"), Support Vector Machine, Artificial Neural Network, Decision Tree, Ensemble Methods – boosting, linear regression, K-Nearest Neighbor, etc. Recently, there are a few studies on predicting the mechanical properties of stainless steel using data-science techniques[6)-10)]. In the present study, however, RF was employed as a machine learning- method, because some recent studies have shown it performs best in predicting material properties from features of the materials[10)]. However, no studies have yet predicted the mechanical properties of stainless steel based on other material properties.

In present study, the authors predicted tensile strength and uniform elongation from elastic modulus, proportion limit, 0.2% proof stress, etc. by applying RF to material test results of stainless steel which were collected by Rasmussen[5)]. The aim of the present study is to clarify prediction accuracy of RF by comparing values predicted by RF with ones predicted by prediction equations[5)]. Also, the present study aims to show the effect of explanatory variables used in machine learning on the prediction results and to demonstrate the effect of steel grade and loading direction on root mean square error (hereafter abbreviated to "RMSE").

2. Rasmussen's constitutive equation

Although Ramberg-Osgood curve[3)] has widely used as a constitutive equation of stainless steel, it has been pointed out that the curve overestimates stress beyond 0.2% proof stress for a given strain. Rasmussen proposed a constitutive equation in order to improve its fitness for the stress-strain curve in a range beyond 0.2% proof stress. This equation consists of a general (1st) Ramberg-Osgood curve up to 0.2% proof stress and the 2nd Ramberg-Osgood curve in the range beyond 0.2% proof stress, as shown in Fig.1. 2nd Ramberg-Osgood curve connects smoothly to 1st one at 0.2% proof stress and passes the tensile strength. A constitutive equation proposed by Rasmussen is expressed as follows:

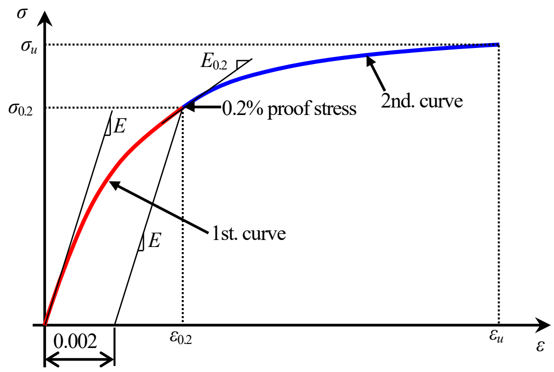

Fig.1 Schematic illustration of constitutive equation proposed by Rasmussen

$$\varepsilon = \begin{cases} \dfrac{\sigma}{E} + 0.002\left(\dfrac{\sigma}{\sigma_{0.2}}\right)^n & for\ \sigma \le \sigma_{0.2} \\ \dfrac{\sigma - \sigma_{0.2}}{E_{0.2}} + \varepsilon_u\left(\dfrac{\sigma - \sigma_{0.2}}{\sigma_u - \sigma_{0.2}}\right)^m + \varepsilon_{0.2} & for\ \sigma > \sigma_{0.2} \end{cases} \quad (1)$$

Where ε is the strain, σ is the stress, E is the elastic modulus, $\sigma_{0.2}$ is 0.2% proof stress, and n is the hardening exponent, which is expressed by using 0.01% proof stress $\sigma_{0.01}$, as follow.

$$n = \frac{\ln(0.05)}{\ln(\sigma_{0.01}/\sigma_{0.2})} \quad (2)$$

In addition, $\varepsilon_{0.2}$ is the total strain at 0.2% proof stress, ε_u is the uniform elongation, σ_u is the tensile strength, and the hardening exponent of 2nd Ramberg-Osgood curve m and the tangent modulus at 0.2% proof stress are expressed by Eqs 3 and 4, respectively.

$$E_{0.2} = \frac{E\sigma_{0.2}}{\sigma_{0.2} + 0.002nE} \quad (3)$$

$$m = 1 + 3.5\frac{\sigma_{0.2}}{\sigma_u} \quad (4)$$

Where, Eq. 4 is an equation obtained by trial and error so that the ratio of $\sigma_{0.2}$ and σ_u corresponds with the stress-strain curve.

3. Data sets and prediction methods

3・1 Data sets for machine-learning

Rasmussen proposed prediction equations which can estimate the tensile strength σ_u and the uniform elongation ε_u from the dimensionless 0.2% proof stress $\sigma_{0.2}/E$ and the hardening exponent n by collecting and analyzing material test results of stainless steel[5)]. The authors employed thirteen and sixteen tensile coupon test results of austenitic stainless steel UNS30403 (JIS SUS304L) with regard to longitudinal and transverse directions, respectively, fifteen and sixteen tensile coupon test results of austenitic stainless steel UNS31603 (JIS SUS316L) with regard to longitudinal and transverse directions, respectively, nineteen and twenty-nine tensile coupon test results of duplex stainless steel UNS31803 (JIS SUS329J3L) with regard to longitudinal and transverse directions, respectively, and twelve tensile coupon test results of ferritic stainless steel UNS43000 (JIS SUS430) and 3Cr12 steel as data sets for machine-learning.

3・2 Prediction equations proposed by Rasmussen

Based on material test results of stainless steel, Rasmussen has proposed a prediction equation for the tensile strength σ_u expressed as follows[5)]:

$$\frac{\sigma_{0.2}}{\sigma_u} = \frac{0.2+158e}{1-0.0375(n-5)} \tag{5}$$

Hardening exponent n of Eq.5 is employed 5 for austenitic and duplex stainless steels and 12 for ferritic stainless steel.

Rasmussen also has proposed a prediction equation of the uniform elongation ε_u from yield ratio $\sigma_{0.2}/\sigma_u$ by regression analysis. The prediction equation is given as follow:

$$\varepsilon_u = 1-\frac{\sigma_{0.2}}{\sigma_u} \tag{6}$$

That is, the tensile strength σ_u is able to be predicted from elastic modulus E, 0.2% proof stress $\sigma_{0.2}$ and hardening exponent n by using Eq.5. Subsequently, the uniform elongation ε_u is able to be predicted from $\sigma_{0.2}$ and σ_u by using Eq.6.

3・3 RF

The inputs for machine learning using the RF program were basically raw E, $\sigma_{0.2}$, n, σ_u and ε_u, and σ_u and ε_u, were predicted from E, $\sigma_{0.2}$, n and σ_u. This study employed 1000 decision trees, its depth was fixed at 10, and the seed value for random sampling was set at 2 as a constant value. Leave-One-Out cross validation was used, which repeats the evaluation of a model by replacing training data with validating data.

4. Prediction results

This chapter shows prediction of tensile strength σ_u and the uniform elongation ε_u which are objective variables from elastic modulus E, hardening exponent n and 0.2% proof stress $\sigma_{0.2}$ which are explanatory variables. Prediction accuracies of σ_u and ε_u by RF are clarified by comparing with σ_u and ε_u predicted by Rasmussen's equations. In addition to E, n and $\sigma_{0.2}$, this chapter demonstrates the effect of the number of explanatory variables on prediction accuracies of σ_u and ε_u by considering steel grade, loading direction (longitudinal / transverse directions), plate thickness t, and 1% proof stress σ_1 as explanatory variables. Finally, this chapter relatively compares the RMSE of tensile strength and uniform elongation for each steel type and loading direction.

4・1 Comparison predicted values with tested ones

In case of three explanatory variables, Fig.2 shows a relationship between yield ratio $\sigma_{0.2}/\sigma_u$ obtained from the material test and its predicted value by using Eq.5 and RF. In Fig.2, in addition to, lines indicating 0%, plus or minus (±)5% and ±10% error compared to test results are shown between test results and values predicted by using Eq.5 and RF, to highlight the difference between the test results and predicted values.

From Fig.2, with regard to austenitic and duplex stainless steels, Eq.5 is able to predict tensile strength at about 10 – 20 % higher. On the other hand, RF is able to predict it within ±10%. In case of ferritic stainless steel, some values of tensile strength predicted by Eq.5 shows almost its half value obtained from tensile test. In contrast to Eq.5, RF is able to predict tensile strength within ±20%. However, in case of ferritic stainless steel, prediction accuracy of tensile strength by RF tends to decrease compared to austenitic and duplex stainless steels, because tensile strength σ_u does not

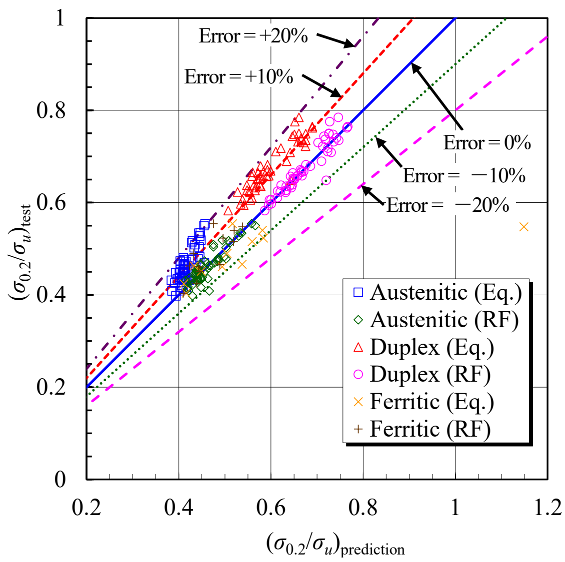

Fig.2 Comparison of tensile strength predicted by Eq.5 and RF

always have a good correlation with elastic modulus E, 0.2% proof stress $\sigma_{0.2}$ and hardening exponent n. Therefore, it is concluded that tensile strength predicted by RF exhibits higher accuracy than that predicted by Eq.5.

Fig.3 compares prediction values of uniform elongation by Eq.6 and RF with the test results. In Fig.3, in addition to, lines indicating 0%, ±5% and ±10% error compared to test results are shown between test results and values predicted by using Eq.6 and RF.

From Fig.3, regardless of prediction method, scatter of uniform elongation is greater than that of tensile strength, because uniform elongation ε_u does not have a good correlation with elastic modulus E, 0.2% proof stress $\sigma_{0.2}$ and tensile strength σ_u. In case of austenitic and duplex stainless steels, uniform elongation values predicted by Eq.6 and RF have same error compared to the test results. However, in case of ferritic stainless steels, uniform elongation predicted by RF has a much smaller error than Eq.6.

4・2　Effect of explanatory variable

Rasmussen has collected material test results on steel grade such as UNS30403, UNS31603, etc., loading direction (longitudinal / transverse directions), plate thickness t and 1% proof stress σ_1, besides elastic modulus E, hardening exponent n and 0.2% proof stress $\sigma_{0.2}$. High-precision prediction of tensile strength and uniform elongation would be expected by adding these four parameters to explanatory variables. In practical design, these parameters are able to be easily obtained from mill certificates except for 1% proof stress. Therefore, the authors obtained a prediction equation for tensile strength σ_u (N/mm^2) given in Eq.7 from a linear regression analysis on one hundred twenty test data including steel grade and loading direction.

$$\begin{aligned}\sigma_u &= 379.4 - 24.4x - 1.284y + 0.6253t \\ &\quad + 0.2095E - 2.279n + 0.1553\sigma_{0.2} + 0.58\sigma_{1.0}\end{aligned} \tag{7}$$

Where 1, 2, 3, 4 and 5 as value of x means for UNS30403, UNS31603, UNS31803, UNS43000 and 3Cr12, respectively. And, y = 1 and 2 indicates that the loading direction is parallel to longitudinal and transverse directions, respectively. Moreover, t is the plate thickness (mm), E is the elastic modulus (kN/mm^2), n is the hardening exponent, $\sigma_{0.2}$ is 0.2% proof stress (N/mm^2) and σ_1 is 1% proof stress (N/mm^2).

A prediction equation of uniform elongation ε_u (%) was obtained from a linear regression analysis on one hundred twenty test data as with case of tensile strength. The prediction equation is expressed as follow:

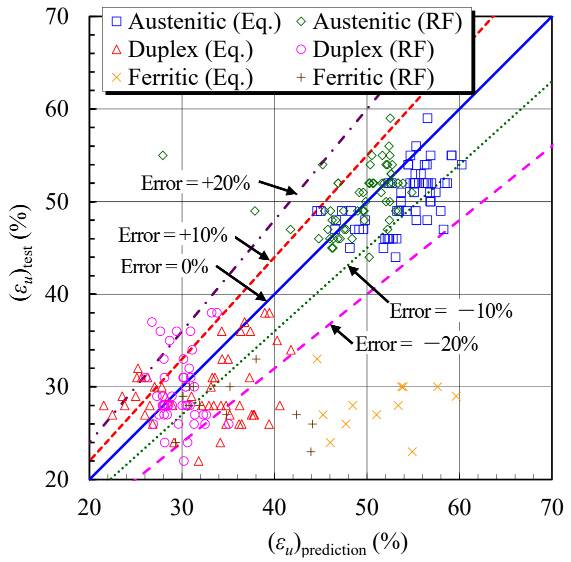

Fig.3 Comparison of uniform elongation predicted by Eq.6 and RF

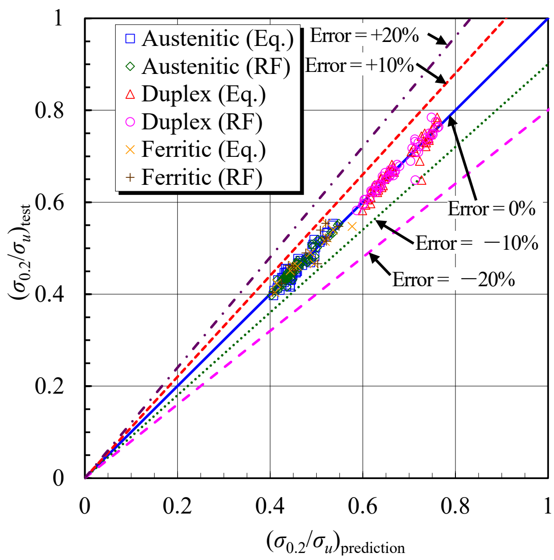

Fig.4 Comparison of tensile strength predicted by Eq.7 and RF

$$\begin{aligned}\varepsilon_u &= 68.0 - 5.3x - 0.305y + 0.3789t + 0.00896E \\ &\quad - 0.125n + 0.0704\sigma_{0.2} - 0.58\sigma_{1.0}\end{aligned} \tag{8}$$

In addition to prediction using Eqs.7 and 8, tensile strength and uniform elongation were also predicted by RF which was considered steel grade, loading direction, plate thickness, elastic modulus, hardening exponent, 0.2% proof stress and 1% proof stress as explanatory variables.

Fig.4 compares prediction values of tensile strength by Eq.7 and RF with the test results. In Fig.4, in addition to, lines indicating 0%, ±5% and ±10% error compared to test results are shown between test results and values predicted by using Eq.7 and RF.

Fig.4 demonstrates that prediction accuracy of Eq.7 is dramatically improved by adding seven parameters such as steel grade, loading direction, etc. in comparison with tensile strength predicted by Eq.5 as shown in Fig.2. Therefore, it is found that ultimate strength of stainless steel has strong correlation with steel grade, plate thickness and 1% proof stress besides elastic modulus and hardening exponent. On the other hand, although prediction accuracy of tensile strength by RF was not improved as much as prediction accuracy of Eq.7, RF by considering 7 parameters was observed slight improvement of prediction accuracy compared to RF by using 3 parameters. Both Eq.7 and RF by using 7 parameters are able to predict tensile strength in an error within 10%, whereas Eq.7 is more complicated than Eq.5.

Fig.5 compares uniform elongation predicted by Eq.8 with that obtained from test results. Despite addition of explanatory variables, with regard to duplex and ferritic stainless steels, the error of uniform elongation predicted by Eq.8 still larger than that of tensile strength by Eq.7, because uniform elongation does not always correlate with elastic modulus and tensile strength. However, Fig.5 shows the effectiveness by adding explanatory variables, because prediction accuracy is dramatically improved by using Eq.8 in comparison with Eq.6 which is employed three parameters. On the other hand, although uniform elongation predicted by RF which is employed 7 parameters shows slightly small error in comparison with that predicted by RF which is used 3 parameters, improvement effect of accuracy by adding explanatory variables to RF is small compared to the case by using Eq.8. As well as Eq.6, in practical use, Eq.8 is needed to be used carefully because it is complicated.

4・3 RMSE

Fig.6 shows RMSE values of tensile strength for each steel type and loading direction. Numbers described in lateral axis mean steel grade and loading direction, as defined in Table 1. In a legend of Fig.6, "RF (3)" and "RF(7)" indicate RF which are employed three and seven explanatory variables respectively.

From Fig. 6, RMSE of the values predicted by Eq.5 are prominent compared to that of the values predicted by Eq.7 and RF. In case of ferritic stainless steel, RMSE of the values predicted by Eq.5 exceeds 100×10^{-3} N/mm^2. However, by addition of explanatory variables, RMSE of the values predicted by Eq.7 dramatically decreases in comparison with that of the values predicted by Eq.5. Also, RMSE of the values predicted by Eq.7 is less than that of the values predicted by RF which is used three explanatory variables. On the other hand, without regard to steel grade and loading direction, RMSE of the values predicted by RF which is

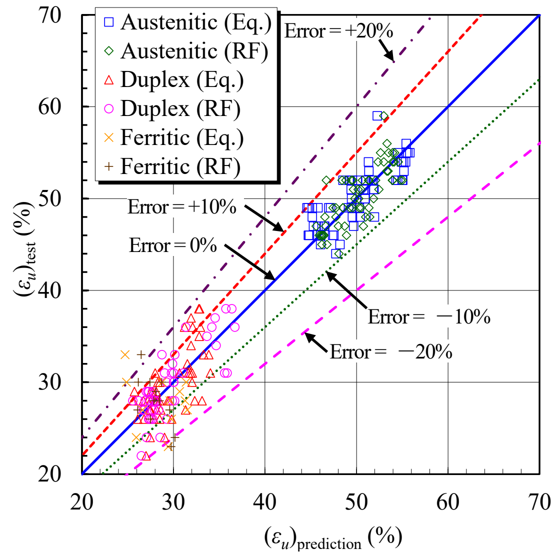

Fig.5 Comparison of uniform elongation predicted by Eq.8 and RF

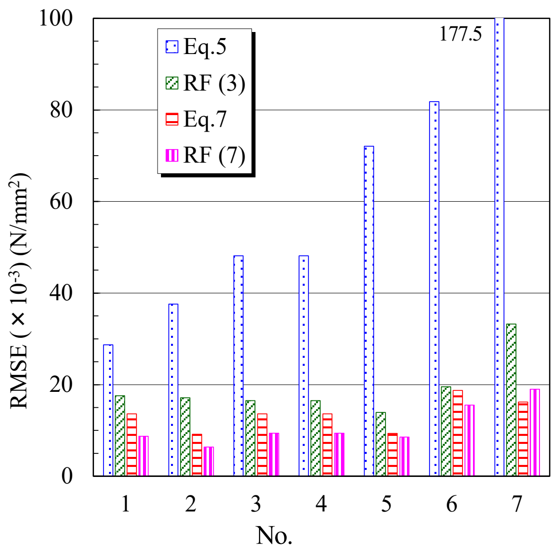

Fig.6 Root mean square error of tensile strength

Table 1 Definition of relationship between number, steel grade and loading direction

No.	Steel grade	Loading direcition
1	UNS30403	Longitudinal
2	UNS30403	Transverse
3	UNS31603	Longitudinal
4	UNS31603	Transverse
5	UNS31803	Longitudinal
6	UNS31803	Transverse
7	UNS43000, 3Cr12	—

employed three explanatory variables is less than 40 × 10^{-3} N/mm^2. RMSE of the values predicted by RF which is employed seven explanatory variables is slightly smaller than that of values predicted by Eq.7 except for ferritic stainless steel. Therefore, it is found that RF has excellent prediction accuracy in comparison with Eqs.5 and 7.

Regarding the effect of steel grade and loading direction, RMSE of the values predicted by Eq.5 is prominent for duplex and ferritic stainless steels and that for transverse direction tends to cause higher value. However, RMSE of the values predicted by RF which is used three explanatory variables shows insignificant difference depending on steel grade and loading direction except for ferritic stainless steel. In addition, RMSE of the values predicted by Eq.7 and RF which is employed seven explanatory variables do not exceed 20 × 10^{-3} N/mm^2. Therefore, they have insignificant differences depending on steel grade and loading direction.

RMSE values of uniform elongation for each steel type and loading direction are shown in Fig.7, in the same way as Fig.6.

From Fig.7, as with RMSE of tensile strength, that of uniform elongation predicted by RF is generally smaller than that of one predicted by Eqs.6 and 8. Also, it is found that addition of explanatory variables improves the prediction accuracy because RMSEs of the values predicted by Eq.8 and RF which is used seven explanatory variables are smaller than those of the values predicted Eq.6 and RF which is used three explanatory variables. The ratios of RMSE calculated from Eq.8 to Eq.6 are generally smaller than those of one calculated from Eq.7 to Eq.5. This seems to be due to weak correlation between uniform elongation and explanatory variables.

Regarding the effect of steel grade, RMSE values for ferritic stainless steel are prominent in comparison with those for austenitic and duplex stainless steels, whereas RMSE values for austenitic and duplex stainless steels are almost equivalent. On the other hand, RMSEs exhibit insignificant differences depending on loading direction without regard to prediction method.

５. Conclusions

The present study predicted tensile strength and uniform elongation of stainless steels by applying RF which is one of machine learning- method to data analysis of existing material test results. In addition, prediction results were compared with the results using prediction equations

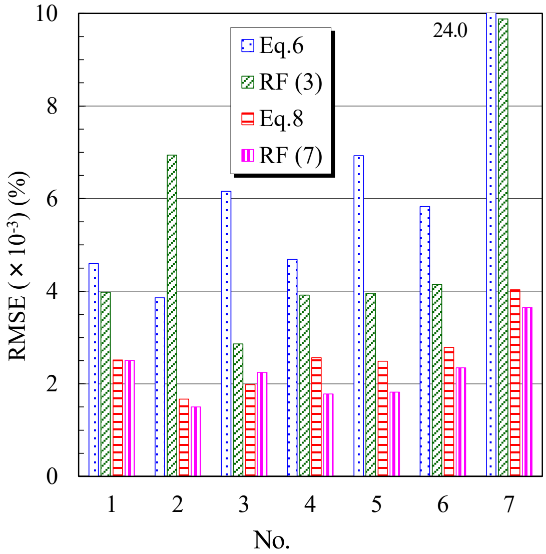

Fig.7 Root mean square error of uniform elongation

proposed by Rasmussen. Moreover, the present study demonstrated the effect of the number of explanatory variables on prediction accuracies by considering steel grade, loading direction, plate thickness, and 1% proof stress, besides elastic modulus, hardening exponent and 0.2% proof stress. The obtained results can be summarized as follows:

(1) Prediction accuracy of uniform elongation was lower than that of tensile strength without regard to prediction method.

(2) RF exhibited generally high prediction accuracy compared to prediction equations based on regression analysis.

(3) For both prediction equations and RF, prediction accuracy was improved by adding explanatory variables.

(4) Prediction accuracy for ferritic stainless steel tended to be lower than for austenitic and duplex stainless steel.

(5) Insignificant differences of predicted values were observed depending on loading directions when RF is used as a prediction method.

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