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Original Article

Statistical analysis of parameter estimation of a probabilistic crack initiation model for Alloy 182 weld considering right-censored data and the covariate effect

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A B S T R A C T

To ensure the structural integrity of nuclear power plants, it is essential to predict the lifetime of Alloy 182 weld, which is used for welding in nuclear reactors. The lifetime of Alloy 182 weld is directly related to the crack initiation time. Owing to the large time scatter in most crack initiation tests, a probabilistic model, such as the Weibull distribution, has mainly been adopted for prediction. However, since statistically more advanced methods than current typical methods may be applied, we suggest a statistical procedure for parameter estimation of the crack initiation time of Alloy 182 weld, considering right-censored data and the covariate effect. Furthermore, we suggest a procedure for uncertainty evaluation of the estimators based on the bootstrap method. The suggested statistical procedure can be applied not only to Alloy 182 weld but also to any material degradation data set including right-censored data with covariate effect.

1. Introduction

To ensure the structural integrity of nuclear power plants, it is essential to predict the initiation time of primary water stress corrosion cracking (PWSCC) [1–3]. For Alloy 182 welds, the prediction becomes more crucial than that for Alloy 600 base metal, since the crack growth rate of Alloy 182 weld was reported to be five times higher than that of Alloy 600 [2].

However, it is almost impossible to obtain a formula that can accurately predict the initiation time of cracking due to the complexity and large number of factors in the PWSCC initiation mechanism. Moreover, most laboratory experiments showed that there was nonnegligible scatter in the PWSCC initiation time, although all specimens were well controlled in the same test conditions (e.g., same temperature and tensile stress, etc.) [4]. These facts made it difficult to develop deterministic PWSCC initiation models and justified an approach to develop probabilistic PWSCC initiation models that can quantitatively consider the time scatter. Accordingly, the extremely low probability of rupture (xLPR) code, developed for regulatory purposes by the Nuclear Regulatory Commission and the Electric Power Research Institute, adopted the probabilistic approach rather than the deterministic approach [5].

The amount of PWSCC data is limited, because it is very difficult and time consuming to obtain such data. Therefore, it is quite important to develop a method for determining the best model using limited data. In this respect, it appears that statistically more advanced methods than current typical methods may be applied in the development of a probabilistic cracking model with limited data. More specifically, a more general and efficient parameter estimation method for the probabilistic crack initiation model should be considered. For example, the xLPR code development team suggested a stress exponent value for the Alloy 182 PWSCC model using aggregated laboratory test data [4]. However, in the parameter (i.e., stress exponent) estimation process in their work [4], right-censored data were not considered. This implies that they only considered PWSCC cracking time data and that NO-PWSCC suspended time data were neglected, where NO-PWSCC suspended time means that the specimen showed no cracking until

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that time and was not censored after that time (i.e., right-censored data). Additionally, the curve fitting method, which was used in the study by Troyer et al [4], is not likely to be the best approach for parameter estimation, as the maximum likelihood estimation (MLE) method is known as the most efficient approach in most cases [6–8].

Therefore, considering the above issues, we suggest an advanced statistical procedure for parameter estimation of PWSCC initiation time of Alloy 182 weld. Furthermore, we suggest a procedure for uncertainty evaluation of the estimators based on the bootstrap method [9].

2. Model development

2.1. PWSCC data

As mentioned previously, the xLPR code development team presented aggregated results for several Alloy 182 PWSCC initiation tests conducted until 2015 [4]. To quantify the stress level applied to the PWSCC specimens, only the test data for tensile load or pressurized capsule specimens were selected. The PWSCC data were normalized at 325°C using the Arrhenius reaction rate rule with 185 kJ/mol of activation energy for Alloy 182 crack initiation [4]. Fig. 1 shows a total of 59 PWSCC cracking time data points extracted from a graph from the study by Troyer et al [4] using the graph digitizer program *GetData* [10].

In the study by Troyer et al [4], a power function was assumed to model the effect of true stress on crack initiation time as follows:

$$t_i \propto (\textit{Applied True Stress})^n, \quad (1)$$

where t_i is the deterministic crack initiation time and n is the stress exponent. The stress exponent n is the parameter that indicates how sensitive the crack initiation time is to the applied true stress. Through curve fitting, the xLPR team suggested $n = -5$, as shown in Fig. 1 (in fact, power fitting suggested $n = -5.2$; however, the engineering approach was adopted [4]).

As mentioned in the Introduction, the xLPR team estimated the stress exponent value without considering the NO-PWSCC suspended time data.

Fig. 2 shows 55 NO-PWSCC suspended time data points that were not considered in the stress exponent estimation, as well as 59 PWSCC cracking time data points. In this graph, the x-axis was changed to the *stress ratio* instead of the true stress, which is shown in Fig. 1. The stress ratio is a dimensionless number indicating the amount of stress that was applied, compared with the yield strength of the material at the testing temperature [4]. Thus, the stress ratio r is defined as follows:

$$r = \frac{\text{Applied True Stress}}{\text{Yield Strength at Test Temperature}}. \quad (2)$$

2.2. Determination of model form

Before carrying out the proposed parameter estimation method considering the NO-PWSCC data shown in Fig. 2, the PWSCC initiation time model should be determined. According to the extremal types theorem [11] and the fundamental mechanism of crack initiation (i.e., weakest link behavior [12]), the Weibull distribution is an appropriate probabilistic model of crack initiation time, at least at macroscopic scale [8]. Therefore, we assumed the Weibull distribution as a base model. Equations (3) and (4) are the cumulative distribution function (CDF) and hazard function of the Weibull distribution, respectively:

$$F(t;\beta,\eta) = 1 - \exp\left[-\left(\frac{t}{\eta}\right)^{\beta}\right] \quad (3)$$

$$\lambda(t;\beta,\eta) = \frac{\beta t^{\beta-1}}{\eta^{\beta}}, \quad (4)$$

where, $t \geq 0$ is the time variable, $\beta > 0$ is the shape parameter, and $\eta > 0$ is the scale parameter of the Weibull distribution. In general, the shape parameter β is considered to be a material constant and not to be affected by surrounding conditions [5,13,14]. On the contrary, the scale parameter η can be affected by several PWSCC related factors such as the applied stress [5].

If $\beta < 1$, the hazard function of the Weibull distribution, which is generally interpreted as the cracking rate, is a monotonically

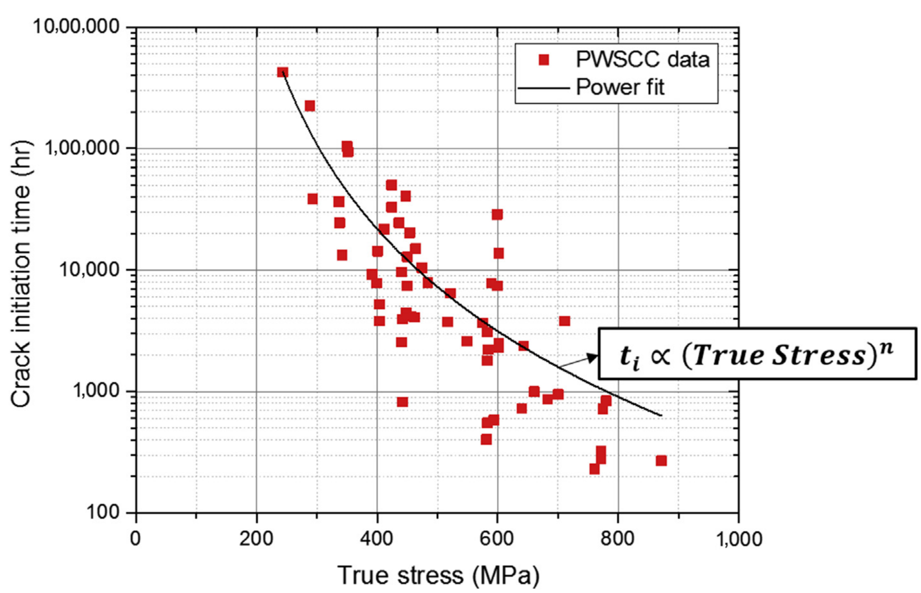

Fig. 1. Alloy 182 PWSCC initiation test results: crack initiation time versus true stress; data from the study by Troyer et al [4]. PWSCC, primary water stress corrosion cracking.

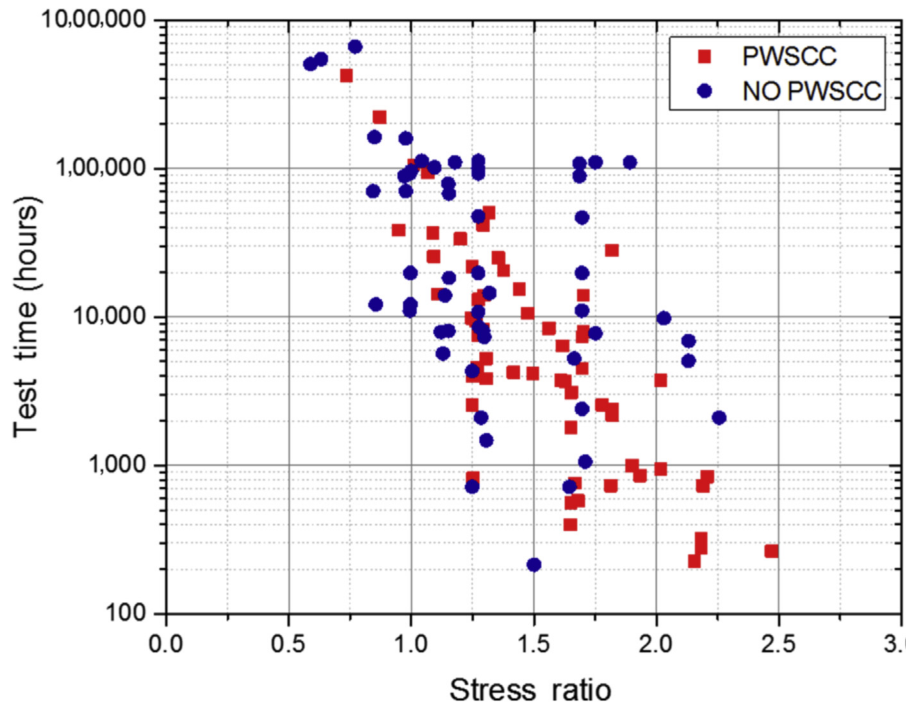

Fig. 2. Alloy 182 PWSCC initiation test results: test time versus stress ratio, data from the study by Troyer et al [4]. PWSCC, primary water stress corrosion cracking.

decreasing function of time. If $\beta > 1$, it is monotonically increasing. In this case, it can be considered that the material undergoes aging [12]. Whereas, the scale parameter η implies a characteristic time, which is a quantile when the Weibull CDF reaches the value 0.632 approximately (i.e., $1-e^{-1} \approx 0.632$) [7,12].

3. Model parameter estimation

We can obtain two types of information from the PWSCC data in Fig. 2:

- The variation of crack initiation probability with time
- The variation of crack initiation probability with stress ratio.

Since the Weibull distribution, which was assumed as the PWSCC model, has a time variable, the variation of crack initiation probability with the stress ratio becomes a *covariate* effect [15]. In this case, it is complicated to estimate the model parameters due to the right-censored data in the given PWSCC data. One of the simplest approaches to this problem is to remove the covariate effect from the data. For example, it is possible to model the covariate effect through data fitting (as applied in the study by Troyer et al [4]) and normalize data to eliminate the covariate effect. However, this approach has a limitation in handling right-censored data.

Thus, we suggest the following approach. It is first assumed that the Weibull scale parameter η has a power function relationship with respect to the stress ratio r, as follows:

$$\eta = \eta_y r^{n_r}, \tag{5}$$

where, η_y is the scale parameter of the Weibull distribution when the stress ratio $r = 1$ (i.e., applied stress is equal to the yield strength at testing temperature) and n_r is the stress ratio exponent. The above assumption differentiates our model from that in the study by Troyer et al [4] in the following two respects:

- The stress ratio r (instead of the true stress) is an independent variable.
- The Weibull scale parameter η (instead of the deterministic crack initiation time t_i) is a function of the stress ratio r.

However, we emphasize that our methodology can be applied to any type of right-censored data considering the covariate effect.

Substituting Eq. (5) into Eq. (3) yields the CDF and probability density function of the PWSCC model as follows:

$$F\left(t, r; \beta, \eta_y, n_r\right) = 1 - \exp\left[-\left(\frac{t}{\eta_y r^{n_r}}\right)^{\beta}\right], \tag{6}$$

$$f\left(t, r; \beta, \eta_y, n_r\right) = \frac{\beta}{\eta_y r^{n_r}}\left(\frac{t}{\eta_y r^{n_r}}\right)^{\beta-1} \exp\left[-\left(\frac{t}{\eta_y r^{n_r}}\right)^{\beta}\right]. \tag{7}$$

Since, in most cases, the MLE method is the most efficient estimation method [6,7], we perform parameter estimation using this method. For the exact (i.e., PWSCC cracking time) and right-censored (i.e., NO-PWSCC suspended time) data, the likelihood function can be expressed as follows [16]:

$$L\left(\beta, \eta_y, n\right) = \prod_{i=1}^{C}\left[f\left(t_{ci}, r_{ci}; \beta, \eta_y, n_r\right)\right] \prod_{j=1}^{S}\left[1 - F\left(t_{sj}, r_{sj}; \beta, \eta_y, n_r\right)\right], \tag{8}$$

where,C is the number of PWSCC cracking time data points (=59), t_{Ci} is the i^{th} PWSCC cracking time, r_{Ci} is the stress ratio for the i^{th} PWSCC data point, S is the number of NO-PWSCC suspended time data points (=55), t_{Sj} is the j^{th} NO-PWSCC suspended time point, and r_{sj} is the stress ratio for the j^{th} NO-PWSCC data point.

Since the logarithm function is a monotonically increasing function, it is convenient to use a log-likelihood to find the maximum likelihood estimates. Taking logarithms on both sides of Eq. (8) and substituting Eq. (6) and (7) into Eq. (8) yields the following log-likelihood function:

$$
\begin{aligned}
l\left(\beta,\eta_y,n_r\right) &= \ln L\left(\beta,\eta_y,n_r\right)\\
&= \sum_{i=1}^{C}\left[\ln\beta-\ln\eta_y-n_r\ln r_{ci}+(\beta-1)\right.\\
&\qquad\left.\left(\ln t_{ci}-\ln\eta_y-n_r\ln r_{ci}\right)-\left(\frac{t_{ci}}{\eta_y r_{ci}^{n_r}}\right)^{\beta}\right]+\\
&\qquad\sum_{j=1}^{S}\left[-\left(\frac{t_{sj}}{\eta_y r_{sj}^{n_r}}\right)^{\beta}\right].
\end{aligned}
\tag{9}
$$

The estimate is a parameter vector maximizing Eq. (9) (i.e., $\text{argmax}_{(\beta,\eta_y,n_r)}[l(\beta,\eta_y,n_r)]$), which can be calculated by solving the following partial differential equations:

$$
\begin{cases}
\dfrac{\partial}{\partial\beta}l\left(\beta,\eta_y,n_r\right)=0\\[2ex]
\dfrac{\partial}{\partial\eta_y}l\left(\beta,\eta_y,n_r\right)=0\\[2ex]
\dfrac{\partial}{\partial n_r}l\left(\beta,\eta_y,n_r\right)=0.
\end{cases}
\tag{10}
$$

The final simultaneous equations are given by substituting Eq. (9) into Eq. (10) as follows:

$$
\begin{cases}
\displaystyle\sum_{i=1}^{C}\left[\frac{1}{\beta}+\ln\left(\frac{t_{ci}}{\eta_y r_{ci}^{n_r}}\right)\left[1-\left(\frac{t_{ci}}{\eta_y r_{ci}^{n_r}}\right)^{\beta}\right]\right]+\sum_{j=1}^{S}\left[-\left(\frac{t_{sj}}{\eta_y r_{sj}^{n_r}}\right)^{\beta}\ln\left(\frac{t_{sj}}{\eta_y r_{sj}^{n_r}}\right)\right]=0\\[3ex]
\displaystyle\sum_{i=1}^{C}\left[-\frac{\beta}{\eta_y}+\left(\frac{\beta}{\eta_y}\right)\left(\frac{t_{ci}}{\eta_y r_{ci}^{n_r}}\right)^{\beta}\right]+\sum_{j=1}^{S}\left[\left(\frac{\beta}{\eta_y}\right)\left(\frac{t_{sj}}{\eta_y r_{sj}^{n_r}}\right)^{\beta}\right]=0\\[3ex]
\displaystyle\sum_{i=1}^{C}\left[(\beta\ln r_{ci})\left[\left(\frac{t_{ci}}{\eta_y r_{ci}^{n_r}}\right)^{\beta}-1\right]\right]+\sum_{j=1}^{S}\left[(\beta\ln r_{sj})\left(\frac{t_{sj}}{\eta_y r_{sj}^{n_r}}\right)^{\beta}\right]=0.
\end{cases}
\tag{11}
$$

Since Eq. (11) is a nonlinear system of equations, it is almost impossible to find an analytical solution. Therefore, we adopted a numerical approach using the *fsolve* function in MATLAB, version. R2015b. The estimates using this numerical method are given by:

- β estimate: $\hat{\beta}=0.6153$
- η_y estimate: $\hat{\eta}_y=325,280\ h$
- n_r estimate: $\hat{n}_r=-5.4583$

It is surprising that the value of $\hat{\beta}$ is less than unity, because this implies a monotonically decreasing rate of crack initiation (i.e., decreasing hazard function) with time. Moreover, it is contrary to the precedent study on Weibull shape parameters for Alloy 600 and 182 materials [5,13,14,17]. We speculate that this is due to the *data aggregation* effect [18]. It has already been reported that an underestimation phenomenon for the Weibull shape parameter could occur because of data aggregation when local data sets have similar shape parameters but different scale parameters [18]. Additionally, it is known that there is larger uncertainty in the shape parameter estimation than in the scale parameter estimation [7,8]. Therefore, it is preferable to set $\beta=3$, as in the earlier research [5,13,14], rather than to use the estimate (i.e., $\hat{\beta}=0.6153$) as the PWSCC model parameter.

On the other hand, it is reasonable to use $\hat{\eta}_y=325,280\ h$ and $\hat{n}_r=-5.4583$ as the model parameters. Fig. 3 shows the physical meaning of each estimate. As mentioned earlier, η_y implies the characteristic time of the Weibull distribution when the stress ratio $r=1$. Thus, the $\hat{\eta}(r)$ curve is not the best fitting curve for all data points, but rather the estimation of the characteristic time line at which the cumulative cracking probability reaches approximately 63.2%. If the value of $\hat{\eta}_y$ becomes larger, it can be anticipated that the $\hat{\eta}(r)$ curve (black solid line in Fig. 3) will be shifted upward; in the opposite case, the $\hat{\eta}(r)$ curve will be shifted downward. As far as $\hat{n}_r$ is concerned, the gradient of the $\hat{\eta}(r)$ curve will decrease when the value of $\hat{n}_r$ approaches zero.

4. Uncertainty evaluation of estimators

In the previous section, the PWSCC model parameters were estimated considering the censored data and covariate effect. Then, it is necessary to evaluate the uncertainty of the estimated model parameters. Since the estimation of β was not reliable, uncertainty evaluation for $\hat{\beta}$ appears to be meaningless. Therefore, we focus on the procedure of uncertainty evaluation for $\hat{\eta}_y$.

4.1. Stress ratio normalization

It is now possible to eliminate the covariate (i.e., stress ratio) effect in the PWSCC data, because the value of stress ratio exponent n_r was estimated in the previous section. As shown in Fig. 4, in order to normalize the i^{th} PWSCC data point (r_i,t_i) to the given reference stress ratio line (e.g., $r=r_0=1.0$), the following relationship is assumed based on Eq. (5):

$$
\left(\frac{t_i}{t_{0i}}\right)=\left(\frac{r_i}{r_0}\right)^{n_r}\quad\text{or}\quad t_{0i}=\frac{t_i}{\left(\frac{r_i}{r_0}\right)^{n_r}}=t_i\left(\frac{r_i}{r_0}\right)^{-n_r},
\tag{12}
$$

where, r_0 is the reference stress ratio and t_{0i} is the i^{th} PWSCC time data point after the stress ratio normalization. After the above data shifting has been carried out for all PWSCC points, we can treat the normalized PWSCC data as having no covariate effect.

4.2. Empirical cumulative distribution function

We now draw the empirical CDF from the normalized data. However, because of the presence of right-censored data, the empirical CDF cannot be drawn simply by assigning the same probability mass to each data point. In 1958, Kaplan and Meier [19]

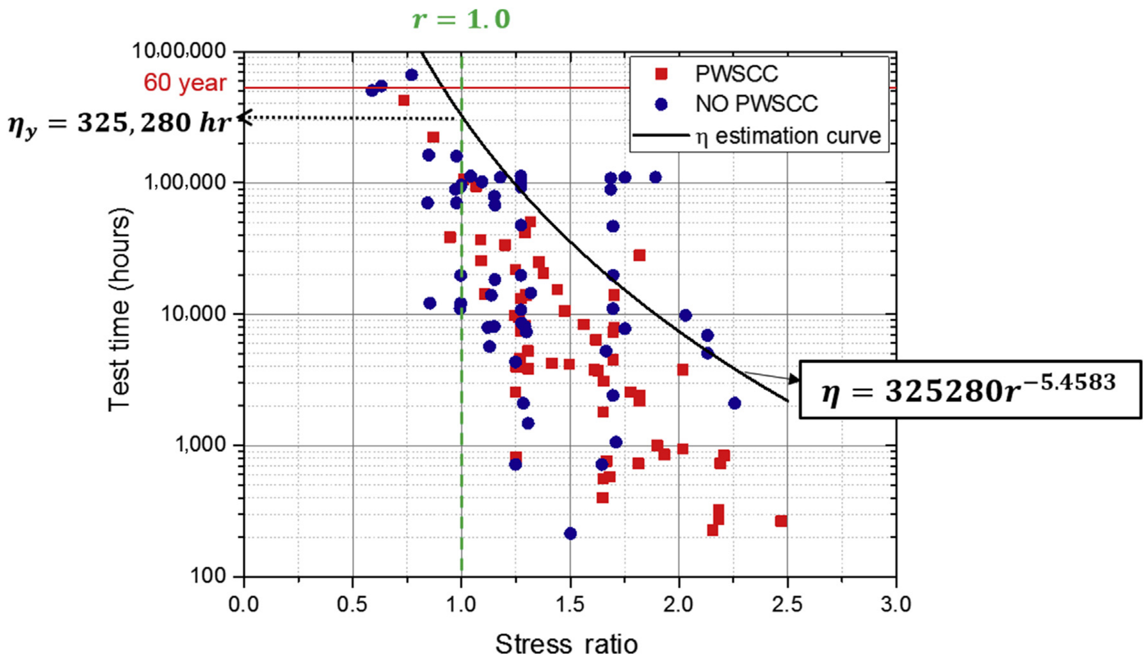

Fig. 3. Parameter estimation results and physical meanings of $\eta(r)$, η_y, and n_r. PWSCC, primary water stress corrosion cracking.

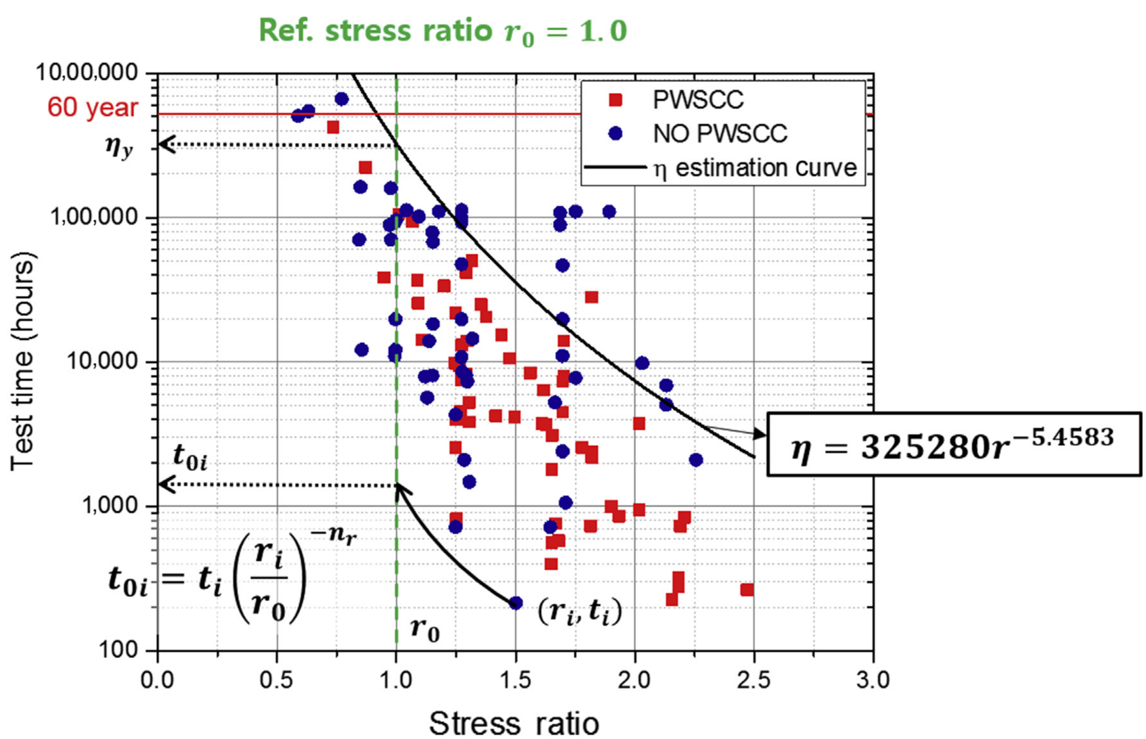

Fig. 4. Graphical illustration of stress ratio normalization for i^{th} data point to the reference stress ratio $r_0 = 1.0$. PWSCC, primary water stress corrosion cracking.

studied this problem and developed a method (the Kaplan–Meier method) that is based on an algorithm related to the hazard rate at each data point [19]. Using the Kaplan–Meier method, the black solid line in Fig. 5 is the empirical CDF drawn from the normalized data when $r_0 = 1$.

4.3. Bootstrapping

The bootstrap method [9] enables uncertainty evaluation of the estimators with only experimental data and without assuming that the estimator will follow a specific distribution (e.g., normal distribution). Therefore, it can be applied even when a parametric interval estimation is impossible or requires a complicated formula, provided that there are sufficient testing data.

After the empirical CDF is obtained, we can calculate the confidence interval of the estimators using a bootstrap method. Fig. 6 schematically illustrates the procedures of bootstrapping.

1) It is first assumed that the random variable T in Fig. 6 follows the distribution of the inherent crack initiation time. As noted

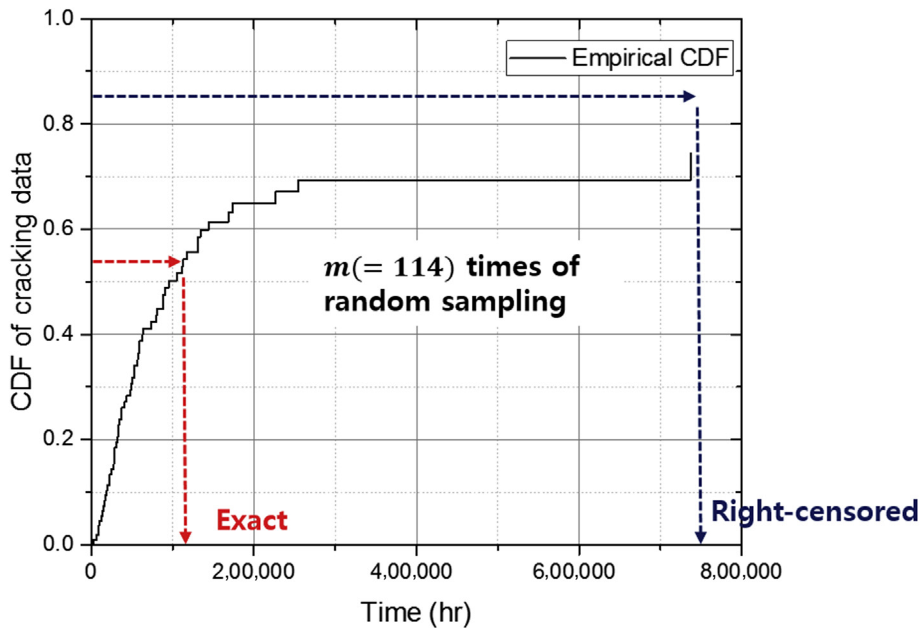

Fig. 5. Empirical CDF of the PWSCC data with the reference stress ratio $r_0 = 1$. CDF, cumulative distribution function; PWSCC, primary water stress corrosion cracking.

previously, at least on macroscopic scale, we can assume that the random variable T follows the Weibull distribution.

2) The *sample set* is obtained by drawing a random sample of size m from the population. In this case, the sample set consists of 59 PWSCC data points and 55 NO-PWSCC data points; that is, $m = 59 + 55 = 114$.
3) The *bootstrap sample set* is obtained by further drawing a random sample of size m with replacement from the sample set. We note that if there is right-censored data, as in this case, a more delicate resampling process is required, as follows [20]:
   i. We generate a random number uniformly distributed in [0,1].
   ii. If the generated random number is less than or equal to the maximum value of the empirical CDF, we take the quantile of the empirical CDF according to the random number. Then, the resulting quantile value is treated as an exact data point in the bootstrap sample set (see the red dashed line in Fig. 5).
   iii. If the generated random number is greater than the maximum value of the empirical CDF, we take the quantile at the maximum point of the empirical CDF. Then, the resulting quantile value is treated as a right-censored data point in the bootstrap sample set (see the blue dashed line in Fig. 5).
   iv. We repeat steps (i) and (ii) or (iii), $m(=114)$ times to generate the other elements in the bootstrap sample set.
4) We repeat step (3) B times to generate the other bootstrap sample sets. We note that the value of B should be sufficiently large. Generally, a value of more than 10,000 is recommended [9]; we select 10,000 as the B value.
5) We calculate the estimates for all bootstrap sample sets. In our case, we used the 2-parameter MLE method.
6) We finally obtain the bootstrap confidence interval (or variance) of the estimators from the set of bootstrap estimates.

Using the above bootstrap procedure, we draw the scatter plot of the bootstrap estimates with $r_0 = 1$, as shown in Fig. 7.

The blue dot in Fig. 7 is the sample set estimate (i.e., estimated from the sample set), the red dots are the bootstrap estimates when the bootstrap sample sets were re-sampled using the empirical CDF

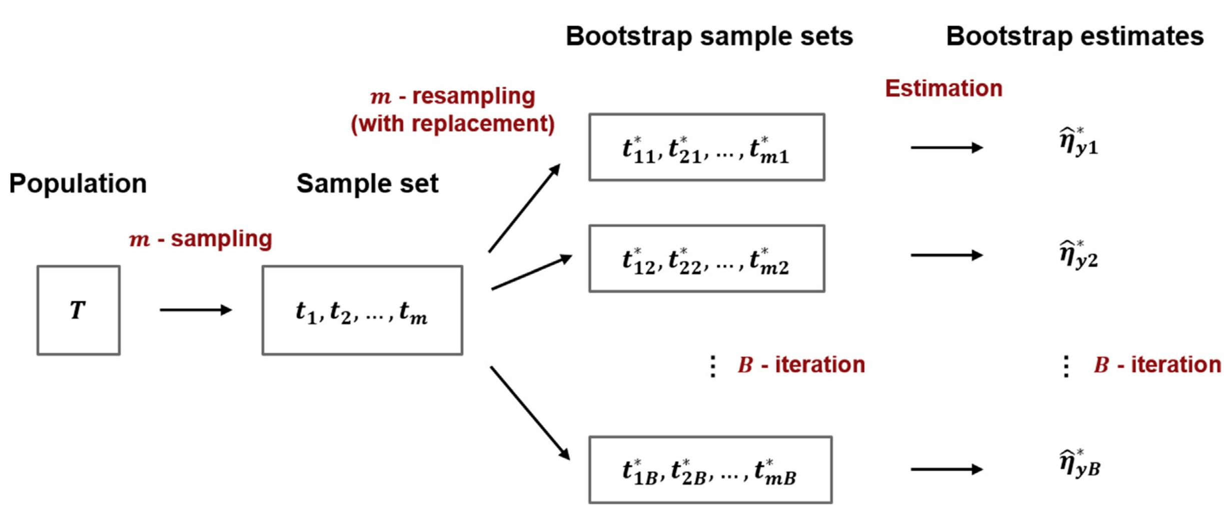

Fig. 6. Schematic illustration of bootstrapping.

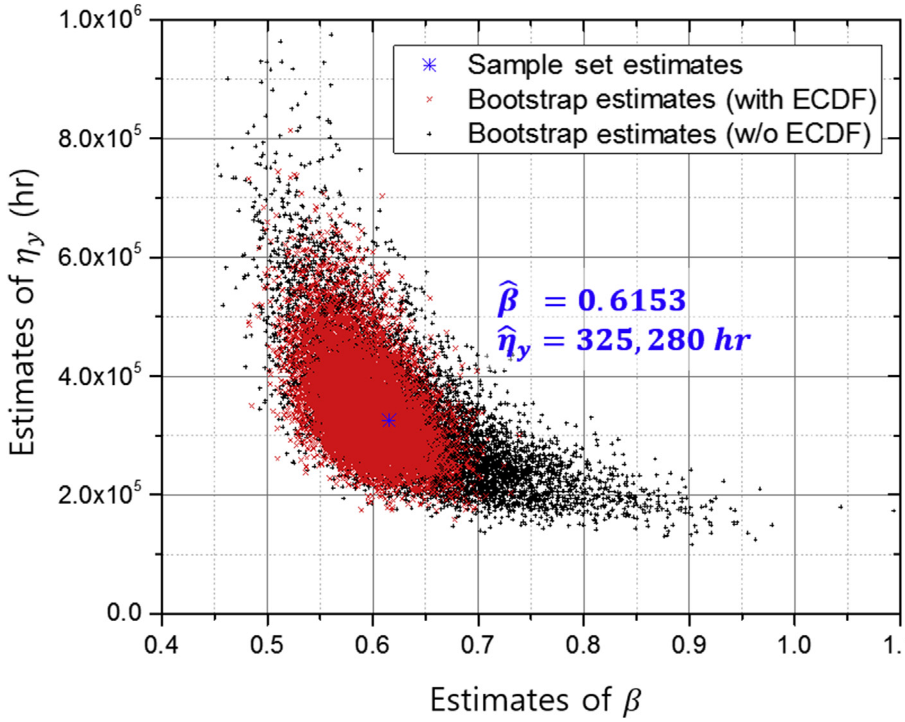

Fig. 7. Scatter plot of β and η_y estimates when the reference stress ratio $r_0 = 1$. ECDF, empirical cumulative distribution function.

in step (3); and the black dots are the bootstrap estimates when the bootstrap sample sets were re-sampled *without* using the empirical CDF (i.e., resampled directly from the sample set). It is likely that the dispersion of red dots is smaller than that of black dots. This is possibly due to the smaller probability of producing right-censored data for the resampling process when the empirical CDF is used. For a quantitative comparison, Table 1 represents the 5th and 95th percentiles of the bootstrap estimates of $\hat{\eta}_y$. It is confirmed that the length of the 90% bootstrap confidence interval (i.e., 95th percentile estimate−5th percentile estimate) is shorter when the resampling process is performed with the empirical CDF. Therefore, in accordance with earlier research [20], in this study we adopted the confidence interval obtained with the empirical CDF.

However, as mentioned earlier, the PWSCC data used here are an aggregation of test results; thus, βcould be underestimated [18]. Therefore, the bootstrap confidence interval for $\hat{\beta}$ is of little importance. Thus, we considered the confidence interval for $\hat{\eta}_y$ only.

Fig. 8 shows an interpretation of the resulting confidence interval. If the stress exponent $r = 1$ and the Weibull shape parameter $\beta = 3$ are assumed, we can draw the prediction curve of the cumulative cracking probability (black solid line in Fig. 8), 5% lower bound, and 95% upper bound (black dash lines in Fig. 8). It can be pessimistically anticipated that the cumulative cracking probability will be about 5% after 10 years of operation, or it can be optimistically anticipated that the cracking probability will be about 70% after 60 years of operation. However, we note that this interpretation should be validated through the plant PWSCC data [21].

To obtain the confidence interval for $\hat{\eta}$ for stress ratios other than $r = 1$, we repeat the procedure described above. Fig. 9 shows the bootstrap confidence interval for $\hat{\eta}$ when the stress ratio varies between 0.75 and 2.5.

It is likely that the 90% bootstrap confidence interval for $\hat{\eta}(r)$ is considerably narrow. Such a narrow confidence interval appears to be due to the relatively large number of data points (i.e., 114 ea.) used for bootstrapping.

5. Conclusions

This work was intended to provide statistical insight for developing probabilistic crack initiation models. We suggested an advanced statistical procedure of parameter estimation and a procedure for uncertainty evaluation of the estimators in the probabilistic crack initiation model. Fig. 10 summarizes the suggested procedure. The following conclusions can be drawn:

- A statistical method of parameter estimation and uncertainty evaluation was proposed considering right-censored data and the covariate effect. We illustrated and analyzed the proposed method with real data (Alloy 182 PWSCC initiation test data). This method can be used for various applications with right-censoring along with a covariate.

Table 1
Results of the bootstrapping when the reference stress ratio $r_0 = 1$.

Parameter	Sample set estimate (hr)	Resampling process	Bootstrap estimate (hr)		Length of 90% confidence interval (hr)
			5%	95%	
η_y	325,280	W/O empirical CDF	203,170	520,220	317,050
		With empirical CDF	246,080	486,330	240,250

CDF, cumulative distribution function.

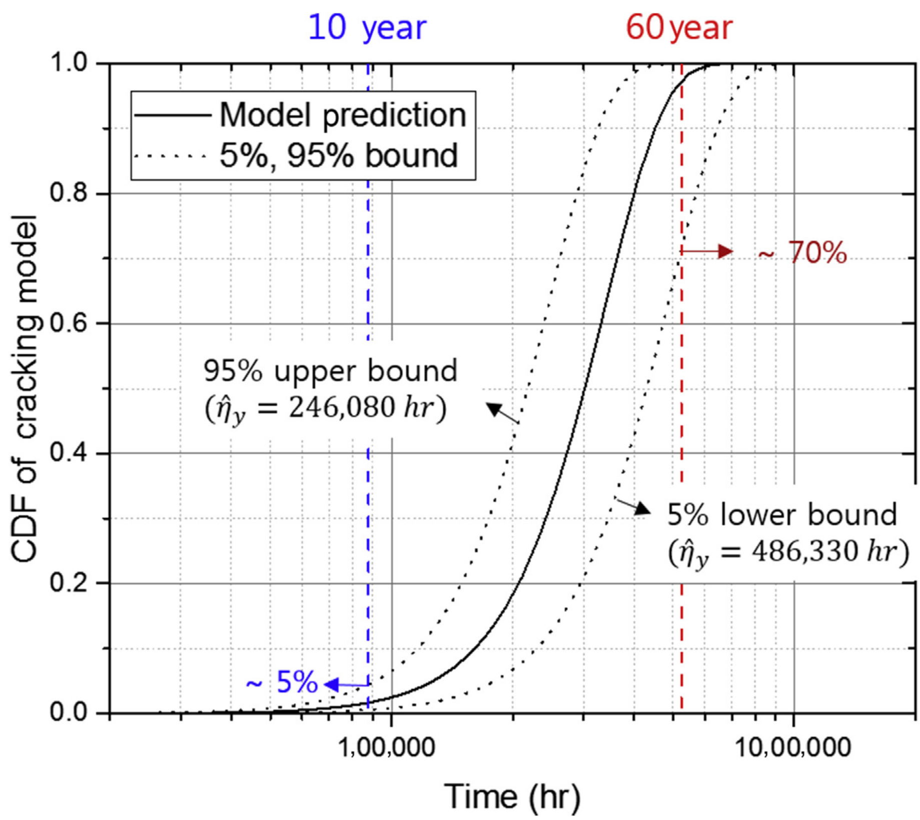

Fig. 8. CDF of the PWSCC model with the result of confidence interval for $\hat{\eta}_y$, when the reference stress ratio $r_0 = 1$. CDF, cumulative distribution function; PWSCC, primary water stress corrosion cracking.

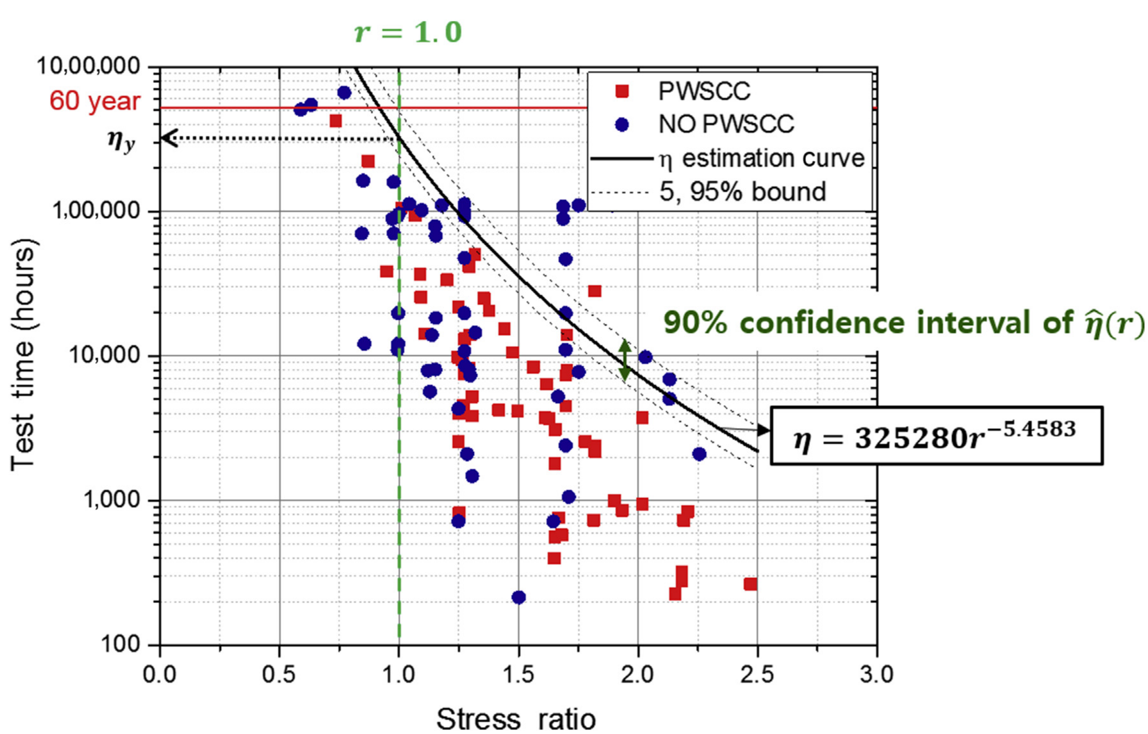

Fig. 9. Ninety percent confidence interval of $\hat{\eta}(r)$ when the stress ratio ranges from 0.75 to 2.5. PWSCC, primary water stress corrosion cracking.

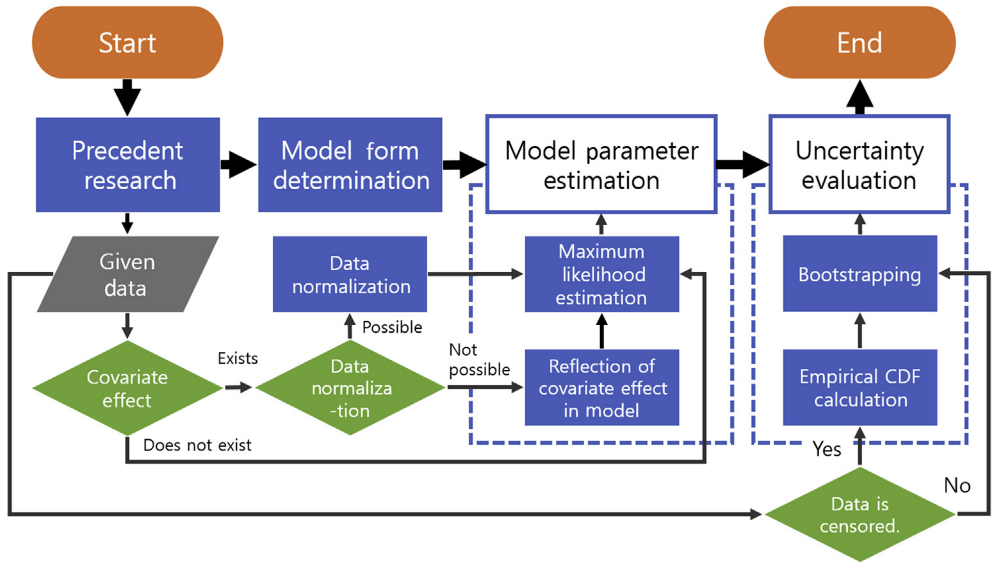

Fig. 10. Flow chart of the suggested parameter estimation and uncertainty evaluation procedure. CDF, cumulative distribution function.

- When estimating the Weibull model parameters from an aggregated data set, we confirmed that the shape parameter could be underestimated.
- The uncertainty of the estimated model parameters was evaluated by a bootstrap method that uses the empirical CDF for resampling.

Conflicts of interest

All authors have no conflicts of interest to declare.

Acknowledgments

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