Transactions of the Korean Nuclear Society Autumn Meeting
Changwon, Korea, October 24-25, 2024

Evaluation of Parameters in High-temperature Deformation Creep Model of Fuel Cladding using Bayesian Optimization

Do-Hyen Song[a], Chang-Hwan Shin[b], Sung-Uk Lee[b], Hyo-Chan Kim[b], Byoung-Jae Kim[a*]
[a]*Mechanical Engineering, Chungnam Nat'l Univ., 99, Daehak-ro, Yuseong-gu, Daejeon*
[b]*Korea Atomic Energy Research Institute, 111, Daedeok-daero 989beon-gil, Yuseong-gu, Daejeon*
[*]*Corresponding author: bjkim@cnu.ac.kr*

Keywords : zircaloy-4 cladding, creep parameters, rupture data, bayesian optimization

1. Introduction

Among various reactor accidents, in the case of a Loss of Coolant Accident(LOCA), the primary cause of flow blockage during reflooding of the emergency core cooling system is high-temperature deformation of cladding, such as expansion and rupture. In particular, circumferential deformation has a significant impact, and extensive research has been conducted on this topic. The equation for circumferential creep of cladding is expressed based on the Arrhenius equation and is given by Equation (1).

$$\dot{\varepsilon}_\theta = A_\theta \exp\left(-\frac{Q}{RT}\right)\sigma^n \tag{1}$$

Here, $\dot{\varepsilon}$ is steady-state creep rate, A is structure parameter, Q is activation energy, R is gas constant, T is the absolute temperature, σ is stress, and n is stress exponent. The three parameters of the creep model, A, n, and Q, are empirically determined through steady-state creep test conducted at a constant temperature. However, a creep test is time-consuming and costly because it requires observing the rupture process and obtaining real-time deformation data. In contrast, a burst test conducted under trainsient conditions provides rupture data and requires less time and cost compared to creep test.

This study aimed to derive the creep model utilizing not real-time deformation data from a creep test, but rupture data obtained from a burst test. Accordingly, the three parameters of the creep model were optimized utilizing the rupture data for the Zircaloy-4 cladding.

2. Creep Parameters Optimization

Various techniques exist for parameter optimization. Bayesian Optimization differs from Grid Search and Random Search by using previous search results to determine the next search. This study utilized Bayesian Optimization to more efficiently find the optimal values.

Steady-state creep test has been conducted using various methods, among which the model and parameters proposed by Rosinger's axial tensile test are the most widely used. Rosinger's creep parameters are provided in Table I[1], and this study focused only on the α-phase. Since Rosinger's model provides axial creep parameters, these were converted to circumferential creep parameters by using the anisotropy coefficients according to Hill's definition[2], as shown in Equation (2).

$$A_\theta = \left(\frac{F+G}{4} + H\right)^{\frac{n-1}{2}} (0.5F+H)(F+G)^{-\frac{n+1}{2}} A_z \tag{2}$$

To calculate circumferential creep from axial creep parameters, optimized anisotropy coefficients[3] were used, as shown in Table II. Additionally, to take into account initial elastic and thermal deformation, the material properties of Zircaloy[4] were incorporated.

A Python code was developed based on burst test data from NUREG-0630[5] and Massih's study[6]. Using the Scikit-learn library, the datasets were divided into Training and Test sets for optimization and validation.

Optimization was performed using the Mean Absolute Percentage Error (MAPE) as the performance evaluation criterion. The error was calculated by comparing the experimental rupture time with the algorithm-predicted rupture time, where the predicted rupture time is defined as the time when the algorithm-predicted strain reaches the experimental rupture strain.

Table I: Rosinger's axial creep parameters

T[K]	A_z	n	Q	Phase
900 to 1085	19400	5.89	320000	α

Table II: Anisotropy coefficients

Phase	F	G	H
α	0.54	0.60	0.36

3. Results

Bayesian Optimization was conducted over wide ranges, and creep parameters optimized for the burst test data were obtained. The ranges and the obtained creep parameters are shown in Table III, and as observed, they are not similar to Rosinger's creep parameters. To compare rupture processes, Fig. 1 presents time-strain graphs for data classified into four categories based on rupture time. For experimental data with high heating rates and short rupture times, the rupture process is similar to the Rosinger model. However, for data with lower heating rates and longer rupture times, differences are observed. As shown in Fig. 2, the Rosinger model slightly overestimates the rupture times for data with long rupture times, whereas the optimized model shows a better fit.

The performance evaluation of each model is presented in Table IV. The obtained model presents good performance as it is optimized for the datasets.

Table III: Ranges of optimization and optimized parameters

	Rosinger	Bayesian	Range
A_z	19400	103900	0.01 to 110000
n	5.89	4.056	1 to 12
Q	320000	268500	100 to 1000000

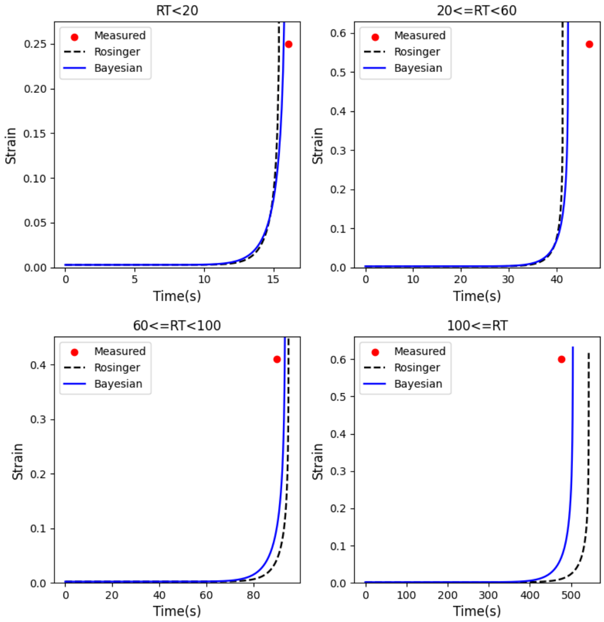

Fig. 1. Time-strain graphs for four randomly selected data categorized based on rupture time.

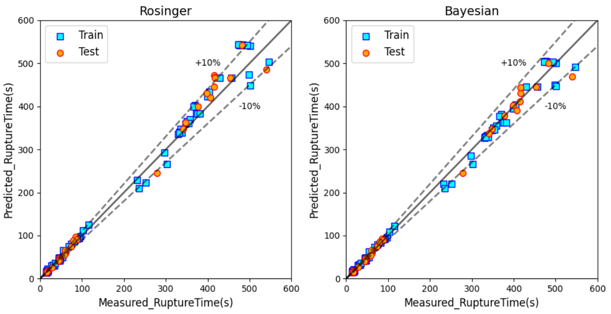

Fig. 2. Comparison of measured values and predicted values for rupture time.

Table IV: Performance evaluation for each creep model

		Rosinger	Bayesian
MAPE(%)	Train	6.4	4.8
	Test	6.8	4.6

4. Conclusions

This study began with the aim of proposing a creep model using only burst test data, bypassing steady-state creep test. Rosinger proposed creep parameters based on quantitative high-temperature deformation data obtained from a creep test. Therefore, the Rosinger model incorporates physical models. The approach in this study, which finds creep parameters that best fit only the rupture data without considering physical models, may not be physically valid. However, because the parameters were obtained through optimization, they can accurately predict the rupture results. The optimized creep parameters showed significant differences from Rosinger's creep parameters; however, the rupture processes were similar when compared. Therefore, it is possible to obtain a creep model through optimization and use it to predict rupture results. This is considered a meaningful result.

For cladding of other materials for which a creep model has not been proposed, it is possible to easily obtain a creep model using only burst test data. However, for a more accurate creep model, steady-state creep test needs to be conducted.

While this method has not been applied to α+β and β-phase data, it could be used in the same way. Additionally, it is expected that this approach can be applied to other materials cladding in the future, enabling the proposal of a creep model without the need for a creep test.

Acknowledgement

This work was supported by the Ministry of Science and ICT of the Republic of Korea.(RS-2022-00144002)

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