The method for the determination of creep cavitation model based on cavity histogram

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Abstract

Most creep rupture is caused by the cavitation at the grain boundary. Hence it is vitally important to develop a creep cavitation model as it is the prerequisite for the development of the creep cavitation rupture model. Due to the experimental difficulty, it is rare to conduct interrupted creep tests to measure cavity growth. However, cavity histograms were more regularly produced and reported to quantitatively report and record the cavity distribution. This research group originally developed such a concept and the procedures to calibrate the cavitation model reversely based on the cavity histogram. This paper reports and summarizes the detailed work in developing the procedure for the calibration of the cavitation models based on the cavity histogram.

Keywords: cavity nucleation and growth; cavity histogram; creep damage; creep strength; high Cr steel.

1. Introduction

Creep causes various microstructural changes and property deteriorations over time; hence the term damages are introduced. Cavitation at grain boundary is, arguably, the most important one, for most of the high temperature structural materials, with regards to structural integrity. However, this has not been adequately appreciated by research communities and high temperature industries [1-4]. Furthermore, from the methodology point of view, some of the practices adopted in the creep continuum damage mechanics do suffer a few fundamental criticisms [1-10] such as: 1). the phenomenological approach does not actually model the creep cavity damage, only its effect was considered; 2). hence, the coupling of creep cavitation damage and deformation is not mechanism based; and 3). the inability to meet the deformation consistency condition in the multi-axial version of creep damage constitutive equations generalized by the Hayhurst approach. Some pioneer and tentative work was carried out and can be seen in [9-18], but not limited by these.

The challenges involved with creep damage mechanics and creep damage models have been analyzed in the literature review such as those shown initially in [2, 3] and formally in [4]; they are:

(1) Characterizing and quantifying creep cavitation and developing damage criterion for parent metal and weld, respectively; experimental work (uniaxial and multi-axial interrupted
creep test) to be carried out or gathered under low stress; cavitation to be quantified, ideally using X-ray micro-tomography. A new damage criterion shall be developed.

(2) Quantifying the microstructural evolutions and their effects on the creep deformation.

(3) Developing and applying the novel creep formulation suitable for a wider range of stress and incorporating the damage criterion developed in (1).

(4) Generalizing uniaxial version into a three-dimensional creep damage model.

Bearing the above thoughts in mind and particularly on the sight of the published 3D synchrotron creep cavity data for high Cr steels [19], a PhD research project was set up to utilize such valuable data [20]. Its success has opened the door for other projects which investigated other alloys and expanded to use other 3-dimensional cavitation data such as those produced by small angle neutron deflection. A series of publication on the cavitation models and creep lifetime prediction were produced [20-28].

In pursuing the above research, we became aware of and utilized the generic creep cavitation model and creep rupture based on area fraction along the grain boundary model proposed and summarized by Riedel in [23].

The application of Riedel’s cavitation model requires 1) a sound understanding of their theories, particularly the theory embodied in the histogram; and 2) a method to determine the values of the five constants in the cavitation model.

It is generally understood and accepted that the best way to obtain the values of the five constants in the cavitation model is through optimization. However, due to the priority of research, we decide to find a practical way to find the numerical answers without having to resort to optimization techniques, although the research group had experience in such a field [29-30].

This paper reports how we devised such practical ways to calibrate the cavitation model practically and quickly.

2. Cavitation model theories

The cavitation nucleation and cavity growth equations are simple enough. The confusion and difficulty are that the cavitation data are typically represented in a histogram; hence an accurate and correct understanding is needed as a prerequisite for the calibration. To understand the concept of histogram, a mathematical textbook such as [31] can be referred to.

The cavitation model theories are summarized in the following. For further details or explanation, see Renversade et al [32] and [4, 24].

The cavity nucleation and cavity growth models are proposed as follows [23]:

\[ J^* = A_2 t^\gamma \]  
\[ \dot{r} = A_1 r^{-\beta} t^{-\alpha} \]  

where \( J^* \) is the nucleation rate of the cavity, \( \dot{r} \) is the non-stationary growth rate of the cavity radius,
$r$, is the individual cavity size and, $t$, is the real time, while $A_1$, $A_2$, $\alpha$, $\beta$, and $\gamma$ are material cavitation constants. It is implicitly assumed that they are not changing during the creep process, but they might be dependent on stress.

Some preliminary explanation of their physical meaning and their significance can be found from literature, such as in [23, 32].

A generic cavity size distribution function at time $t$ was proposed by Riedel [23] and it is shown as:

$$N(R, t) = \frac{A_2}{A_1} R^\beta t^{\alpha+\gamma} \left(1 - \frac{1-\alpha}{1+\beta} \frac{R^{\beta+1}}{A_1 t^{1-\alpha}}\right)^{(\alpha+\gamma)/(1-\alpha)}$$  \hspace{1cm} (2)

where $R$ is cavity radius, $N(R, t)$ is the number of cavitation.

There are five cavitation constants here, namely, $\alpha$, $\beta$, $\gamma$, $A_1$ and $A_2$, in total. Beware of the definition of $R$ in the $N$-$R$ space, as it differs from $r$.

### 3. Determination methods [4, 20, 24] and Experimental data

Mathematically, Equation (1) will uniquely decide Equation (2), and vice versa, so they are equivalent. Hence Xu concluded that:

1. We can determine the values for the cavitation model based on the data in histogram only, and there is no need for any other experimental data such as the direct measurement of the cavity growth rate and/or the change of cavity number over time.
2. The standard approach would be resorting to optimization techniques.
3. Without resorting to optimization, a set of values can be obtained by solving five independent equations, simultaneously, without the optimization, and there are standard procedures for this task.
4. Even more practical, the trial and error method can be used to construct a theoretical histogram, and through comparison of the predicted histogram and experimental data, and this can be very easily achieved by programming with Excel.
5. The known typical values for any variable can be used as a good starting point, which will reduce the order of difficulty and complexity.
6. If the characteristic values for $\alpha$ and $\beta$ have been obtained and the value for $\gamma$ has been suggested for a specific test, then the inner code of the calibration is reduced to find the solution for $A_1$ and $A_2$, given set values of $\alpha$, $\beta$ and $\gamma$. The predicted $r$-$t$ and $N$-$t$ at $t_i$ was used to construct the $N(R, t_i)$.
7. The outside loop can be performed for various values for $\alpha$, $\beta$ and $\gamma$, the sensitivity of the values of $\alpha$, $\beta$, $\gamma$ can be explored afterwards.

This report will focus on the above point 6. The sensitivity study following the above point 7 was conducted but was not reported here in order to concentrate on the former.

The experimental histogram data was chosen for P91 (9Cr–1Mo–V–Nb) steel at 575°C and was shown in Figure 1 [32]. The leftmost and rightmost points were used for our calculation and
illustration. They are $t_i = 10200$ h, respectively, $R_1 = 0.6 \mu m$, $N(R_1, t_f) = 3800$ and $R_2 = 2.4 \mu m$, $N(R_2, t_f) = 1$.

![Image](image_url)

Figure 1. The experimental histogram data for P91 steel [32].

In the cavity size-time space, the maximum cavity $r$ is $r_i$ and $r_j$ corresponding to real time $t_i$ and $t_j$.

Further mathematical equations for calibration are shown as follows:

$$N(R, t_f) = \frac{A_2}{A_1} R^\beta t_f^{1+\gamma} \exp\left(-\frac{1+\gamma}{1+\beta} \frac{R^\beta+1}{A_1}\right)$$  \hspace{1cm} (3)

$$\frac{1}{3} r^3 = A_1 \ln t + C \hspace{1cm} (4.1)$$

$$\frac{1}{3} r_i^3 = A_1 \ln t_i + C \hspace{1cm} (4.1a)$$

$$\frac{1}{3} r_j^3 = A_1 \ln t_j + C \hspace{1cm} (4.1b)$$

$$A_1 = \frac{R_j^3 - R_i^3}{3(\ln t_j - \ln t_i)} \hspace{1cm} (4.1c)$$

$$A_1 = \frac{R_2^3 - R_1^3}{3 \ln (N(R_1, t_f)/R_2^2 N(R_2, t_f)/R_1^2)} \hspace{1cm} (4.2)$$

Substitute $A_1$ into Equation (3) and using the point 2 on the histogram ($R_2 = 2.4 \mu m$, $N(R_2, t_f) = 1$), gives:

$$A_2 = \frac{N(R_2, t_f) A_1}{R_2^2 t_f^2 \exp\left(-2R_2^3/3A_1\right)} \hspace{1cm} (4.3a)$$

Substitute $A_1$ into Equation (3) and using the point 1 ($R_1 = 0.6 \mu m$, $N(R_1, t_f) = 3800$), gives:

$$A_2 = \frac{N(R_1, t_f) A_1}{R_1^2 t_f^2 \exp\left(-2R_1^3/3A_1\right)} \hspace{1cm} (4.3b)$$
3.1 Forward method [20]

The method consists of the following steps and it is implemented via Excel:

1. From a cavity growth point of view, Equation (4.1c) can be used for the determination of \( A_1 \).
2. The first point in \( t-r \) space, it is guessed \( t_i \) for a given \( r_i \), and the second would be \( r_1 = R_2 \) and \( t_j = t_f \). We could take \( r_i = R_1 \), and the \( t_i \) is a guessed value, and it should be relatively very small in comparison with \( t_f \).
3. Then substitute the known \( A_1 \) into Equation (4.3b) to obtain \( A_2 \).
4. Based on the known \( A_1 \) and \( A_2 \), the histogram can be drawn using Equation (3).
5. Based on the difference between the predicted histogram curve with the experimental points, a series of initially estimated time \( t_i \) can be tried out to produce the best fit.
6. The integration constant \( C \) can be found.

In this method, only one point from the histogram is taken for the determination of the constants.

The values found are:
\[ t_0 = 41.367 \text{ h} \text{, then it is found that of } A_1 = 8.2358 \times 10^{-1}, A_2 = 9.95 \times 10^{-5}. \text{ Then it is found that of } C = -2.9938. \]

It is worth reporting that when it is difficult to judge which is the best value for \( t_0 \) when it is around 41 hours, hence there is a small degree of inaccuracy and uncertainty. In this method, only one point, \( R_2 \), from the histogram is directly taken for the determination of the constants. The overall quality of fit is judged in the selection of the trial \( t_i \).

3.2 Xuming Zheng’s method [24]

This method is called a backward method, directly taken two points from the histogram, and it finds the values of \( A_1 \) and \( A_2 \) by solving the two simultaneous Equations (3).

The values are \( \alpha = 1, \beta = 2, \gamma = 1 \). We chose the leftmost and rightmost points for our calculation and illustration, they are: \( t_f = 10200 \text{ h} \), respectively, \( R_1 = 0.6 \mu m, N(R_1, t_f) = 3800 \) and \( R_2 = 2.4 \mu m, N(R_2, t_f) = 1. \)

Specifically,
\[
A_1 = \frac{-2R_1^3 + 2R_2^3}{3\ln(N(R_1, t_f)R_2^2 / N(R_2, t_f)R_1^2)} \tag{4.2}
\]
\[
A_2 = \frac{N(R_2, t_f)A_1}{R_2^2 t_f^2 \exp(-2R_2^3 / 3A_1)} \tag{4.3a}
\]
or
\[
A_2 = \frac{N(R_1, t_f)A_1}{R_1^2 t_f^2 \exp(-2R_1^3 / 3A_1)} \tag{4.3b}
\]

The values found are:
\( A_1 = 8.2358 \times 10^{-1}, A_2 = 9.95 \times 10^{-5} \). Then it is found that of \( C = -2.9938 \) and \( t_0 = 41.367 \text{ h} \).

4. Results and Discussion

The results of the forward method are shown in Figure 2 and Figure 3, while the results of the
backward method are shown in Figure 4 and Figure 5.

Figure 2. The probability density function of cavity equivalent R for P91 by the forward method [27], compared with the experimental histogram data [32].

Figure 2 is displayed the prediction curve by using Equation (3) with the forward method, which fit well with the experimental data. According to the values of $t_0$, $A_1$, C and $A_2$, the curve can be extended to include the condition of the minimum diameter and it is shown in Figure 3.

Figure 3. The prediction curve includes the condition of the minimum diameter [27], compared with the experimental histogram data [32].
Figure 4. The probability density function of cavity equivalent R for P91 by the backward method [27], compared with the experimental histogram data [32].

Figure 4 is displayed the prediction curve by using Equation (3) with the backward method. The curve fit going through the first and last point because these curves are based on these two points to calculate the values of $A_1$, $A_2$ et al. It is not to say that method gives too much weight to those two points. This curve fit better than other curves that are based on another two points for P91 steel. The method is that any two points can be chosen, and the curve can go through these two points necessarily but the curve whether through or nearly the remaining points that is a question. In other words, the trend of the curve is the same as its experimental data and almost points are approaching the curve, this curve based on these two points is the best one. According to the values of $t_0$, $A_1$, $C$ and $A_2$, the curve can be extended to include the condition of the minimum diameter and it is shown in Figure 5.
Figure 5. The prediction curve includes the condition of the minimum diameter [27], compared with the experimental histogram data [32].

Figure 6. The comparison of the accuracy of the two methods [27], compared with the experimental histogram data [32].

Although in the original forward method, the predicted histogram could be constructed using the predicted r-t and N-t relations at t_i, the Excel file we created for the illustration did use N (R, t_i) equation expressed by Equation (3) directly. The intermediate results with various initial t_i under
a set of $\alpha, \beta$ and $\gamma$ are not shown for brevity. The efficiency and convenience of such calculations depend on the parametric coding of the Excel program, the sensitivity study with various $\alpha, \beta$ and $\gamma$ were conducted easily, and they are not reported here either.

The comparison of the two methods is shown in Figure 6. It clearly shows that both methods are capable to produce reasonably accurate results and the difference between them is small by the naked eye. The backward method is better than the forward method due to its directness for determining $A_1$ and $A_2$. The production of $r$-t and $N$-t curves did help to understand the intricate relation of $N (R, t_i)$.

5. Conclusion

As far as the authors are aware of the literature, this is the first time that the method for calibrating a generic cavitation model based on cavity histogram was devised.

The application of the (forward) method enabled the production of the cavitation model, and the derivation of an analytical and explicit creep cavitation damage evolution model. The application of these models will significantly advance the understanding of and modeling of creep damage and rupture.

Parallel to this progress, research on the mesoscopic modeling on the creep deformation and damage has also been undertaken and published [33].

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