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Prediction of Temperature Dependence and Scatter in Fracture Toughness of Pressure Vessel Steel using Nonlocal Damage Models

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Abstract

The pressure vessel and piping components may be subjected to operation in the ductile-to-brittle transition regime of the material due to increase in the transition temperature. This increase can be due to irradiation embrittlement, various other material aging and degradation mechanisms taking place in a nuclear reactor environment. From fracture mechanics point of view, fracture toughness of the material must be adequate to prevent the failure. However, there is considerable scatter observed in the fracture toughness data and the analyst must account for this in the safety analysis. Master curve approach according to ASTM E1921 standard is popularly employed for this purpose. However, it requires the data for transition temperature $T_{0}$ which is dependent upon the specimen geometry and loading configurations employed in the laboratory tests. Its transferability to safety analysis of components is questionable. Towards this objective, the authors have recently developed a nonlocal formulation for the Rousselier’s damage model and combined this with the Beremin’s model to predict the variation of fracture toughness and its scatter in the DBTT regime for the standard compact tension specimens. In this work, application of this new procedure to different types of geometry and loading conditions has been explored.

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Keywords: Fracture toughness master curve; ductile-to-brittle transition; nonlocal formulation

1. Introduction

Most of the safety critical components, such as pressure vessels of nuclear reactors, are made of ferritic grade low-alloy steels. It is widely known that these materials undergo a ductile-to-brittle transition when the temperature is lowered. The ductile-to-brittle transition temperature is very low (of the order -60 to -70 deg. C) for the new and un-irradiated material. However, due to irradiation embrittlement and other material aging and degradation mechanisms, the transition temperature can increase significantly and in the case of an accident scenario such as a loss-of-coolant accident, unstable propagation of cleavage cracks cannot be ruled out. It is

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important to develop a predictive tool to estimate the temperature dependence and scatter in the fracture toughness of these pressure vessel materials in the ductile-to-brittle transition temperature (DBTT) regime. The issues like dependence of the transition temperature $T_0$ on specimen size, geometry, loading conditions etc. which exist in case of master-curve approach [1] may also be resolved through this approach.

Towards this objective, the authors have recently developed a nonlocal formulation for the Rousselier’s damage model [2] and combined this with the Beremin’s model [3] to predict the variation of fracture toughness and its scatter in the DBTT regime for the standard compact tension specimens. In this work, application of this new procedure to different types of geometry and loading conditions has been explored. Experiments have been conducted on different types of specimens such as shallow and deep-notched single-edged-bend specimens, specimens with different size and thickness values etc. The transition temperature $T_0$ has been evaluated using standard procedure and it was observed that $T_0$ is dependent upon the geometry and loading conditions. The combined model has been used to predict the fracture toughness transition curve and the results have been compared with those of experiment.

2. Mesh-independent nonlocal model for ductile fracture

In the earlier works [4-8], the authors have developed a nonlocal formulation of Rousselier’s model [2] using nonlocal damage $d$ as a nodal degree of freedom in the FE mesh. The increment of the nonlocal damage variable $d$ in a material point $\bar{x}$ is mathematically defined as a weighted average of the increment of the local void volume fraction $\dot{f}$ in a domain $\Omega$, i.e.,

$$
\dot{d}(\bar{x}) = \frac{1}{\Psi(\bar{x})} \int \Psi(\bar{y}; \bar{x}) \dot{f}(\bar{y}) d\Omega(\bar{y})
$$

(1)

where $\bar{y}$ is the position vector of the infinitesimally small volume $d\Omega$ and $\Psi(\bar{y}; \bar{x})$ is the Gaussian weight function given by

$$
\Psi(\bar{y}; \bar{x}) = \frac{1}{8\pi^2l^3} \exp \left( -\frac{||\bar{x} - \bar{y}||^2}{4l^2} \right)
$$

(2)

The length parameter $l$ in Eq. (2) determines the size of the volume, which effectively contributes to the nonlocal quantity and is related to the scale of the microstructure. The above integral nonlocal kernel holds the property that the local continuum is retrieved if $l \to 0$. By expanding $\dot{f}(\bar{y})$ in Taylor’s series and substituting in Eq. (1) and doing some algebra, one can obtain the damage diffusion equation as [4-5]

$$
\dot{d} - \dot{f} - C_{\text{length}} \nabla^2 d = 0
$$

(3)

where $C_{\text{length}}$ is the characteristic length parameter of the material. The yield function of the Rousselier’s model [2] is modified by substituting the nonlocal damage $d$ in place of the local ductile void volume fraction $f$ as

$$
\phi = \frac{q}{1-d} + D\sigma_k d \exp \left( -\frac{p}{(1-d)\sigma_k} \right) - R(\varepsilon_{eq}) = 0
$$

(4)

where $D$ and $\sigma_k$ are the parameters of the Rousselier’s model and are constants for a material.

With loading, the void volume fraction evolves from the initial void volume fraction $f_0$ (volume fraction of eligible second phase particles responsible for nucleation of voids upon plastic deformation) in the material. At a critical void volume fraction $f_c$, the voids coalesce with each other and at the final void volume fraction $f_f$, the material loses its stress carrying capability. Hence, the above three void parameters (i.e., $f_0$, $f_c$ and $f_f$) are also the material properties of the damage model.

For solving the boundary value problem of the nonlocal damage continuum, one needs to solve the partial differential equation (3) along with the mechanical equilibrium equation. A FE formulation [4] of the above
process has been implemented in an in-house code and it has been used for analysis of different types of specimens in this work.

3. Beremin’s model for cleavage fracture

Beremin’s model for cleavage fracture is based on the weakest link concept where the probability of fracture can be represented in general as

\[ P_f = 1 - \exp \left( - \int \frac{g(\sigma^i) dV}{V_{\text{ref}}} \right) \]  

(5)

where \( V \) is the volume of the plastically deformed zone (an essential condition for slip induced nucleation of cleavage micro-cracks) in the component, \( V_{\text{ref}} \) is the reference volume which is usually taken as 0.001 mm\(^3\). The function \( g(\sigma^i) \) expresses the probability of failure of an infinitesimal volume of \( dV \) according to the expression

\[ dP_f = g(\sigma^i) \frac{dV}{V_{\text{ref}}} \]  

(6)

where \( \sigma^i \) is the maximum principal stress acting at a material point \( i \) in the plastically deformed region. According to Beremin’s model (which uses Weibull’s statistics for distribution of defects responsible for triggering cleavage according to Griffith’s theory), the form of \( g(\sigma^i) \) is defined as

\[ g(\sigma^i) = \left( \frac{\sigma^i}{\sigma_u} \right)^m \]  

(7)

where \( m \) and \( \sigma_u \) are the Weibull’s shape and size parameters respectively. Using Eq. (7) in Eq. (5), one can obtain the probability of cleavage fracture \( P_f \) at any given loading as

\[ P_f = 1 - \exp \left[ - \left( \frac{\sigma_u}{\sigma_u} \right)^m \right] \]  

(8)

where the loading parameter is defined as the Weibull stress \( \sigma_u \) and is expressed as

\[ \sigma_u = \sqrt[n]{\sum_{i=1}^{n} \left( \frac{\sigma^i}{\sigma_u} \right)^m \frac{V}{V_0}} \]  

(9)

In the present work, Eq. (8) is used to calculate the probability of cleavage fracture of a CT specimen at different loading levels and at different temperatures, where the Weibull stress will be calculated using the stress field ahead of the growing crack using Eq. (9). The nonlocal Rousselier’s damage model has been used to calculate the crack-tip stress field. The effect of evolution of damage (ductile void volume fraction) on the stress field is taken care of by this model and hence, the effect of prior stable crack growth before initiation of cleavage fracture is modeled implicitly through this framework.

4. Results and discussion

In the DBTT regime, the crack-tip experiences a large stress gradient and hence, the ductile crack growth (of the order of few microns) before unstable cleavage fracture cannot be predicted by the local damage models. This is because of the mesh-dependent nature of the results obtained with these models. In order to use fine mesh in the crack-tip and at the same time, to use ductile damage models, the nonlocal formulation of the
Rousselier’s damage model has been used in this work. The results of this model have been demonstrated to be mesh-independent in the earlier works of the authors [4]. Hence, this model along with the Beremin’s model for cleavage fracture has been used to simulate the fracture transition curve for a typical ferritic pressure vessel steel. The true stress-strain curve of the material at different temperatures as used in FE analysis is shown in Fig. 1. Other material properties including the Rousselier’s constants, characteristic length parameter and the void volume fractions (initial, final and at coalescence) are shown in Table-1.

Table-1: Material properties of DIN 22NiMoCr3-7 pressure vessel steel.

| Model parameters | Rousselier’s constants | Void parameters | Char. length parameter | E (Young’s mod. in GPa) | V (Poisson’s ratio) |
|------------------|------------------------|----------------|------------------------|-------------------------|-------------------|
|                  | $D$ $\sigma_k$ (MPa)   | Initial void volume fraction $f_0$ | Void volume fraction at coalescence $f_c$ | Final void volume fraction $f_f$ | Value | 2 | 445 | 0.0003 | 0.05 | 0.3 | 0.05 | 210 | 0.3 |

A standard single-edged cracked specimen, SEB, loaded in three-point bending as shown in Fig. 2 is considered here for the FE analysis. The results of the nonlocal model are shown in Fig. 3. The results of analysis are plotted along with the experimental data and master curves. It can be observed that the model has been able to predict the experimental scatter satisfactorily. The master curve also compares very well with the predictions of the model.

Fig. 1. Stress-strain curve at various temperatures obtained from tensile tests for DIN 22NiMoCr3-7 steel.

Fig. 2. Geometry, dimensions and loading conditions for SEB specimen.

Fig. 3. Predicted fracture toughness scatter and its variation with temperature for the 1T SEB specimen.
Experiments have also been conducted on both shallow-cracked (a/W=0.13) and deeply cracked (a/W=0.53) 1T SEB specimens. The fracture toughness variation in the DBTT regime has been calculated by the model for the shallow-cracked SEB specimen and the results are plotted in Fig. 4 along with experimental data and the master curve data. It can be observed that the FE model has been able to predict the experimental scatter very well in the whole DBTT region. The scatter in fracture toughness as predicted by the model for the deeply cracked specimen has been compared with that of the shallow-cracked specimen in Fig. 5. The fracture toughness values of the shallow-cracked SEB specimen are considerably higher compared to the deeply-cracked SEB specimen and hence, the transition temperature is also lower for the shallow-cracked specimen. Hence, shallow-cracked specimens are less prone to transition compared to deeply-cracked specimens. This is in line with experimental observation. As the crack-tip constraint is lower for the shallow-cracked specimens, the magnitude of crack-tip stress field is lower compared to the deeply-cracked specimens for the same level of loading. This results in lower values of Weibull stresses and hence, the probability of fracture is lower for a given value of $K_{JC}$ loading in case of the shallow-cracked specimen.

In components, the cracks present are usually surface cracks with very small depth compared to the thickness and hence, the data of shallow-cracked specimens are more valid for evaluation of transition temperature in these cases. The master curve as evaluated from deeply-cracked specimens cannot be applied directly for safety evaluation of actual components with very small surface cracks and hence, the modelling technique as presented in this work will be very useful for such situations. Similarly, the effect of specimen size on the fracture toughness variation in the DBTT region was also studied. Fig. 6 presents the predicted results for the 1T, 2T and 4T CT specimens. The 2T and 4T CT specimens are scaled versions of 1T CT specimens with scale factors of 2 and 4 respectively. It can be observed from Fig. 6 that the scatter in the fracture toughness decreases for the specimens with larger dimensions, signifying the increase in the fracture toughness transition temperature. Hence, specimens with larger dimensions are more susceptible to the ductile-to-brittle transition for a given value of loading. This is in line with the experimental observations.

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**Fig. 4.** Predicted fracture toughness scatter in the DBTT region for the shallow cracked SEB specimen.

**Fig. 5.** Effect of crack depth on fracture toughness variation in DBTT regime [shallow vs. deeply cracked SEB].
5. Conclusions

Analysis of ductile-to-brittle transition temperature $T_0$ is very important for safety analysis of critical components in nuclear and other industries where the material may be subjected to operation in the DBTT regime due to degradation in the material properties due to ageing and other phenomena. It may not possible or economic to conduct experiments with wide variety of specimen geometry, size and loading conditions in order to estimate the transition temperature $T_0$ which is required for application of master curve methodology. In this work, it was demonstrated that a combined nonlocal damage model along with the Beremin’s model can satisfactorily predict the scatter in fracture toughness in the DBTT regime for a wide variety of specimen geometry, size and loading conditions with the use of a single set of Weibull parameters. The parameters of the model are transferable across different specimen geometries and hence, these may be used for a reliable safety analysis of critical components in the DBTT regime of ferritic steels.

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