CLEAVAGE FRACTURE ASSESSMENT OF TRANSIENT THERMO-MECHANICAL LOADING SITUATIONS BY LOCAL APPROACH

Johannes Tlatlik, Dieter Siegele

Fraunhofer Institute for Mechanics of Materials IWM, Wöhlerstr. 11, 79108 Freiburg, Germany
johannes.tlatlik@iwm.fraunhofer.de

Abstract

Brittle failure of any nuclear component due to instable propagation of a postulated crack needs to be excluded, and assessed reliably. Currently, cleavage fracture for complex transient loading situations with decreasing temperature and increasing load is analyzed based on isothermal fracture toughness curves with large conservatisms. In this study these transient loading situations were studied experimentally by testing different specimen types (stress conditions) with varying slopes of load versus temperature, and different pre-loads. A probabilistic local approach concept which considers local stress and strain developments, as well as load history, was used to numerically assess cleavage fracture. In all cases the model was able to quantify the fracture probability excellently in a slightly conservative manner. The strong over-conservatism of the Master Curve concept for transient loading was reduced to a tolerable minimum.

Key Words

cleavage fracture, probabilistic model, local approach, Master Curve concept, warm pre-stress effect
## Nomenclature

<table>
<thead>
<tr>
<th>Symbol</th>
<th>Definition</th>
</tr>
</thead>
<tbody>
<tr>
<td>$a_0$</td>
<td>initial crack depth</td>
</tr>
<tr>
<td>$c_1$</td>
<td>material parameter</td>
</tr>
<tr>
<td>$c_2$</td>
<td>material parameter</td>
</tr>
<tr>
<td>$E$</td>
<td>Young's Modulus</td>
</tr>
<tr>
<td>$f_{\text{inst}}$</td>
<td>probability of defect instability</td>
</tr>
<tr>
<td>$f_{\text{nucl}}$</td>
<td>probability of defect nucleation</td>
</tr>
<tr>
<td>$h$</td>
<td>local stress triaxiality</td>
</tr>
<tr>
<td>$h_{\text{global}}$</td>
<td>global stress triaxiality</td>
</tr>
<tr>
<td>$J$</td>
<td>energy release rate</td>
</tr>
<tr>
<td>$J_{\text{eff}}$</td>
<td>effective energy release rate at the crack tip</td>
</tr>
<tr>
<td>$K_J$</td>
<td>crack driving force under mode I loading</td>
</tr>
<tr>
<td>$K_{\text{Jc}}$</td>
<td>critical fracture toughness</td>
</tr>
<tr>
<td>$K_{\text{Jc,1T}}$</td>
<td>standardized critical fracture toughness with 25 mm crack front length</td>
</tr>
<tr>
<td>$m$</td>
<td>material parameter</td>
</tr>
<tr>
<td>$p_f$</td>
<td>probability of failure</td>
</tr>
<tr>
<td>$T$</td>
<td>temperature</td>
</tr>
<tr>
<td>$T_0$</td>
<td>reference temperature where median fracture toughness equals 100 MPa√m</td>
</tr>
<tr>
<td>$T_{0,\text{irr}}$</td>
<td>reference temperature for irradiated materials</td>
</tr>
<tr>
<td>$V$</td>
<td>volume of element</td>
</tr>
<tr>
<td>$W$</td>
<td>width of a specimen</td>
</tr>
<tr>
<td>$\varepsilon_{\text{pl}}$</td>
<td>accumulated equivalent plastic strain</td>
</tr>
<tr>
<td>$\varepsilon_{\text{true}}$</td>
<td>true strain</td>
</tr>
<tr>
<td>$\sigma_i$</td>
<td>maximum principal stress</td>
</tr>
<tr>
<td>$\sigma_{\text{th}}$</td>
<td>threshold stress</td>
</tr>
<tr>
<td>$\sigma_{\text{true}}$</td>
<td>true stress</td>
</tr>
<tr>
<td>$\sigma_u$</td>
<td>Weibull scale parameter</td>
</tr>
<tr>
<td>$\nu$</td>
<td>Poisson's ratio</td>
</tr>
<tr>
<td>CMOD</td>
<td>crack mouth opening displacement</td>
</tr>
<tr>
<td>C(T)</td>
<td>compact (tension)</td>
</tr>
<tr>
<td>FEM</td>
<td>finite-element method</td>
</tr>
<tr>
<td>HRR</td>
<td>Hutchinson, Rice and Rosengren</td>
</tr>
<tr>
<td>LTF</td>
<td>load transient fracture</td>
</tr>
<tr>
<td>SE(B)</td>
<td>single edge-notched (bending)</td>
</tr>
<tr>
<td>WPS</td>
<td>warm pre-stress</td>
</tr>
</tbody>
</table>
1 Introduction

Fracture mechanics assessment of nuclear components is usually performed on the basis of macroscopic concepts by comparing global load parameters such as stress intensity factor or J-Integral with deterministic or probabilistic fracture toughness reference curves belonging to the relevant material (ASME-Code [1][2][3], KTA 3201 [17], or Master-Curve concept [4]). This assessment procedure was derived on the basis of fracture tests at various temperatures but under isothermal conditions, i.e. each single test was performed at constant temperature. On the other hand it is known and experimentally and theoretically determined (i.e. Reed et al. [23]) that pure cooling under constant load does not lead to fracture although the fracture toughness curve of the material is crossed (load cool fracture Fig. 1). Here, the plastic zone ahead of the crack tip does not extend during cooling and therefore no additional energy will be provided to trigger any fracture of particles. Recent work from Siegele et al. [27] and Jacquemoud et al. [14] demonstrates that also different types of load path like load transient fracture also show a profound increase in fracture toughness compared to isothermal testing conditions. Jacquemoud et al. [14] in particular identify the condition of active plasticity as crucial for cleavage fracture, which means the ferrite matrix continuously plasticizes during an increase in load, consequently producing potentially critical microdefects by cracking brittle particles. Rather shallow but still increasing load versus temperature paths that did not show failure experimentally also did not show this active plasticity according to corresponding numerical simulations. As to be shown later, active plasticity is explicitly considered in the following numerical assessment as well.

The mentioned benefit in fracture toughness is well known by literature as the so called warm pre-stress effect (WPS), and it is based on several reasons depending on material and load path (i.e. Nichols [20][21], or Reed and Knott [23][24][25]). One intuitive explanation is for example linked to the fact that the intensified plastic deformation and blunting of the initially sharp crack tip at higher temperatures creates unfavorable cleavage fracture conditions at lower temperatures, “neutralizing” cracks that could lead to failure at lower temperatures and the same load. This has also been identified by Bordet et al. [6] conducting very similar transient load experiments as featured in this study. The WPS-effect through transient load paths was also successfully investigated by Jacquemoud et al. [15], Hure et al. [13], Smith and Garwood [28], or Moinereau et al. [18], proving its relevance and impact on the assessment of fracture toughness for different types of ferritic-bainitic reactor pressure vessel steels. Of special interest regarding this study are results from [15], which emphasizes on proving that active plasticity, the ongoing plastic deformation of the ferric matrix, is a necessary condition for cleavage fracture. This is connected to the nucleation of new microdefects, and will be examined thoroughly in this study as well.

Regarding current fracture assessment, this effect is only considered by KTA 3201 [17] in terms of the so called maximum rule, which states that fracture will not occur if the load achieved during pre-stressing at higher temperatures is not exceeded at lower temperatures, Fig. 1. In practice, most loading transients starting at operating temperature show different slopes dependent on the loading scenario and can also show very small slopes at crossing the fracture toughness curve. For loading transients with decreasing temperature the material zone ahead of the crack tip experiences a plastic deformation at higher temperature which could influence also the fracture probability at low temperatures even for increasing load. There also exists a current attempt to include the WPS-effect in practical French structural integrity assessment, where practical approaches with safety margins and criteria considering pre-loads were established (Chapuliot et al. [7] or Moinereau et al. [19]).

The Master-Curve concept [4] is the most important assessment concept for cleavage fracture on the basis of macroscopic quantities. The experimentally verified strong scatter in fracture
toughness of ferritic steels is explicitly considered in this method, which is motivated by the fact that cleavage fracture is caused by statistically distributed weaknesses (inclusions or precipitates) within the microstructure. On the basis of the calculated stress intensity factor \( K_J \), the probability of failure is determined by the assumption of a three-parameter Weibull distribution. The involved constants are identified accordingly that the median fracture toughness \( K_{jc,\text{med}} \) (50 % fractile) shows the for all ferritic steels identical temperature dependency

\[
K_{jc,\text{med}}(T) = \left( 30 + 70 \exp \left( 0.019 \frac{T-T_0}{\sigma_c} \right) \right) \text{ MPa}\sqrt{\text{m}}
\]

in which the material-, fabrication-, or irradiation-dependent reference temperature \( T_0 \) is the only remaining material parameter. Therefore, a material’s resistance towards cleavage fracture can be described solely by its reference temperature \( T_0 \). Also, this concept is always referred or corrected to a crack front length (specimen thickness) of 25 mm \( K_{jc,1T} \) to consider the fact that the probability of finding larger particles at longer crack fronts increases with increasing specimen thickness.

At higher temperatures, higher loads, or smaller specimen types multiaxial stress effects can cause a loss of constraint resulting in enlarged plastic zones especially towards the specimen sides. Also, it is commonly observed that cleavage fracture initiation originates at some distance ahead of the crack tip which may be located outside of the dominance area of the first term of the Williams expansion of the elastic crack tip stress field or HRR-field. Hence, in this case stress fields at the relevant cleavage fracture initiation sites are not entirely governed by \( K \) or \( J \) causing the experimentally determined fracture toughness not to be a unique material property, but rather a result of this in-plane constraint caused by respective specimen geometries. Wallin [30] proposed a linear correction function of \( T_0 \) to account for the in-plane constraint-effects (T-stress), as well as a consideration of the WPS-effect for load cool fracture load paths in Wallin [29]. However, load transient fracture paths are not considered, and still assessed by the isothermal Master Curve with the supplement of the maximum rule. As an alternative to the T-stress correction [30], Hohe et al. [10] proposed a linear correction of \( T_0 \) by the global stress triaxiality coefficient \( h_{\text{global}} \) which principally agreed with the isothermal experiments and considers both mentioned constraint types. However, for complex transient loading situations a reliable fracture assessment only seems meaningful by the usage of local approach fracture concepts, which inherently conceive the real local mechanical conditions in the area of fracture initiation. The enhanced local probabilistic cleavage fracture model developed by Hohe et al. [11] verifiably describes specimens subjected to these constraint conditions well under isothermal testing conditions, and was used for the subsequent numerical assessment.
Fig. 1: Schematic demonstration of the potential benefit in fracture toughness by choice of different transient load paths compared to isothermal testing conditions.

Probabilistic local approach models allow the direct assessment of cleavage fracture based on the mechanical conditions at the origin of cleavage fracture at the crack tip. The first model of this kind was developed 1983 by the Beremin group [5], and it assumes that cleavage fracture triggering microdefects evolve from the fracture of brittle particles at the onset of plastic deformation of the matrix. Microdefect instability or cleavage initiation is controlled by an instability term (Griffith criterion) that is controlled by defect size and maximum principal stress. More recent and advanced models like proposed from Faleskog et al. [9] additionally take into account the nucleation of microdefects as a linear function of the accumulated plastic strain. Recent studies and models (i.e. Chen et al. [8] have also brought up the relevance of local stress triaxiality controlling whether a microdefect remains sharp or blunts, in the latter case making it uncritical.

In this present study, a local approach model by Hohe et al. [11] was chosen for assessment due to the strong consideration of complex multi-axial stress states at the crack tip, and also an incremental formulation of the model. It could be proven by analyses of fracture experiments that in addition the maximum principal stress the equivalent plastic strain in combination with the stress triaxiality controls the brittle failure, whereas the plastic strain and the stress triaxiality could be connected with the nucleation of critical microdefects. The incremental formulation predicts an incremental increase in fracture probability – therefore considering load histories - opposed to direct formulations which are not suitable for the non-conventional load paths involved in this study. In particular, transient loadpaths were systematically studied in terms of the influence of slope (load versus temperature), pre-load, and stress condition at the crack tip considering C(T) and SE(B) specimens with deep cracks, as well as SE(B) specimens with shallow cracks (Fig.1 red graph). In addition, these loading situations were assessed numerically in terms of cleavage fracture by the local approach model, and compared to the experimental database.
2 Material and Methods
2.1 Material Characterization and Testing Technique

The examined material was the ferritic-bainitic pressure vessel steel 22 NiMoCr 3-7. Conventional isothermal tensile tests in the temperature range of \(-165 °C < T < 200 °C\) were conducted to obtain conventional elastic-plastic material properties. Due to the nature of the following transient investigations, an influence of pre-load at room temperature (+25 °C) on the strength and strain-hardening characteristics of the material was investigated under isothermal quasi-static conditions. Here, a pre-strain of 2, 5, and 10 % respectively was applied to tensile test specimens at 25 °C, and subsequently re-tested at -120 °C. Pre-strain at 25 °C was chosen, because it is the pre-stress temperature of the following transient experiments, and the mentioned strain range of 2-10 % represents the end of the Luders Band and the main region of strain hardening for this material. Furthermore, -120 °C is relevant, because it is near the \(T_0\) reference temperature. It was observed that compared to the conventional stress-strain relation at -120 °C the strain-hardening property of the material is not significantly influenced by the pre-straining at +25 °C apart from the evident parallel shift of the curves, Fig. 2. Therefore, it was assumed that the conventional temperature-dependent elastic-plastic material properties are sufficient as numerical input, which were adequately approximated (Fig. 3 Left), and implemented into a finite-element method (FEM) calculation for assessment. Details of the implementation can be seen in 2.3.

![Fig. 2: Comparison of stress-strain curves of a conventional tensile test at -120 °C and pre-strained tests at +25 °C and re-tested at -120 °C (colored curves are the mean curves of the individually pre-strained specimens)](image)

Fracture mechanics characterization under isothermal conditions according to ASTM E 1921 [4] was conducted, which included C(T)25 and SE(B)-10x18 specimens with a crack depth ratio of \(a_0/W = 0.5\), as well as SE(B)-10x18 specimens with \(a_0/W = 0.13\). This allows a comparison of the achieved fracture toughness upon transient load with the reference condition, as well as a quantification of the constraint-effect under isothermal testing conditions, respectively.

Isothermal fracture toughness reference temperatures of \(T_{0,C(T)}^{iso} = -91 °C\) for C(T) specimens, \(T_{0,SE(B)}^{iso} = -116 °C\), and \(T_{0,SE(B)}^{iso,a/W=0.13} = -115 °C\) were obtained for SE(B) specimens with deep
and shallow cracks, respectively (see Fig. 3). All fracture toughness values above 50 MPa√m are size-corrected to a 25 mm crack front. The $T_0$-shift of $\Delta T_0 = -25 ^\circ C$ of SE(B) specimens is caused by the constraint effect resulting in a lower stress triaxiality at the crack tip region compared to C(T) specimens. Results for the same material from earlier investigations (Hohe et al. [12]) indicate a lower $T_0$-shift of approximately -15 to -20 °C, whereas in the present study the stronger shift might be caused by the higher SE(B) specimen height (18 compared to 10 mm). Moreover, a reduction of crack length ratio to 0.13 causes no further benefit in fracture toughness, whereas this rather unexpected observation can be explained. On the one hand, $T_{0,C(T)}$iso of the C(T) specimens is already lower (-20 °C) than reported in [12]; on the other hand, many tests for SE(B)-10x18 specimens with $a_0/W = 0.13$ were conducted at very low temperatures of < -120 °C. Many tests were even conducted at $T < -140 ^\circ C$ producing fracture toughness values in the lower shelf region below 50 MPa√m showing only elastic material behavior. Essentially, the unnoticeable constraint effect here is most likely linked to the low testing temperatures, and the corresponding low plastic deformation of the material, which is the profound nature of this mechanism. This is strengthened by the fact that by solely observing higher testing temperatures of -90 °C, a slight constraint-effect can be noticed. This explanation is also consistent with experimental data by Ruggieri et al. [26] regarding isothermal fracture mechanics tests with $a_0/W = 0.5$ and 0.15. A strong constraint impact of reducing $a_0/W$ is witnessed here, yet all $a_0/W = 0.15$ tests were performed at temperatures leading to fracture toughness values of $K_{IC} > 100$ MPa√m resulting in sufficient strains to ensure an actual loss of constraint. As mentioned before, this is most likely not the case for the tests with $a_0/W = 0.13$ regarding this study. Higher temperatures would change this as indicated by -90 °C.

![Fig. 3: Left: Approximated temperature dependent elastic-plastic material properties used for the numerical simulations; Right: Fracture mechanics assessment under isothermal conditions for all three specimen types with their corresponding Master Curves (5, 50, and 95 % fractiles).](image)

The experimental testing technique consisted of the identification of the individual transient load paths, Fig. 4 right. The experimental difficulty was that $K_{IC}(T)$ cannot be directly measured or controlled, but only reconstructed from a careful documentation of $CMOD/dt$ and $T/dt$, Fig. 4 left. Furthermore, the desired constant value for $dK_{IC}/dT$ is not equivalent with a constant value of the measureable change in CMOD over time. A detailed overview of the number of specimens and thermomechanical load paths can be seen in Table 1.
In practice, a servohydraulic testing machine and temperature chamber were used in order to conduct crack-mouth opening displacement (CMOD) controlled loading situations and appropriate temperature ramps. In a first step an experimentally achievable constant temperature ramp was determined (cooling rate ≈ -4 °C/min), as well as the thermal correction of the clip-gauge in the temperature range of -175 °C < T < 200 °C for all specimen types. CMOD-measurement was conducted externally with quartz glass rods. In a second step, numerical simulations with the determined temperature ramp and the desired $K_J$-courses were conducted iteratively in order to obtain the necessary CMOD-time courses for the experiments, Fig. 4. These CMOD-courses were implemented experimentally with the previously acquired thermal clip-gauge corrections after an acceptable match of the simulation.

**Fig. 4:** Procedure of determining the transient load paths for experiments.

<table>
<thead>
<tr>
<th>Specimen Type</th>
<th>Nr. of Experiments</th>
<th>$a/W$</th>
<th>Slope $dK_J/dT$</th>
<th>Preload $K_J$</th>
<th>$T_{preload}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>C(T)25</td>
<td>10</td>
<td>0.5</td>
<td>-0.75</td>
<td>165</td>
<td>25</td>
</tr>
<tr>
<td>C(T)25</td>
<td>10</td>
<td>0.5</td>
<td>-0.54</td>
<td>165</td>
<td>25</td>
</tr>
<tr>
<td>C(T)25</td>
<td>10</td>
<td>0.5</td>
<td>-0.35</td>
<td>165</td>
<td>25</td>
</tr>
<tr>
<td>C(T)25</td>
<td>13</td>
<td>0.5</td>
<td>-0.22</td>
<td>165</td>
<td>25</td>
</tr>
<tr>
<td>C(T)25</td>
<td>6</td>
<td>0.5</td>
<td>-0.6</td>
<td>165</td>
<td>25</td>
</tr>
<tr>
<td>C(T)25</td>
<td>6</td>
<td>0.5</td>
<td>-0.6</td>
<td>105</td>
<td>25</td>
</tr>
<tr>
<td>SE(B)10x18</td>
<td>8</td>
<td>0.5</td>
<td>-0.54</td>
<td>165</td>
<td>25</td>
</tr>
<tr>
<td>SE(B)10x18</td>
<td>8</td>
<td>0.13</td>
<td>-0.54</td>
<td>165</td>
<td>25</td>
</tr>
</tbody>
</table>

**Table 1:** Compilation of all thermo-mechanical loading situations.

### 2.2 Local Probabilistic Cleavage Fracture Model

Local probabilistic concepts (local approach) directly assess on the basis of mechanical field variables (stresses and strains) at the origin of cleavage fracture initiation or the immediate vicinity. Fracture criteria have to be formulated upon real micromechanical processes. The great
The advantage of such local approaches is that the assessment is based on the actual physical conditions at the fracture location, and therefore all influencing factors – as well as their interactions – are inherently conceived. For the following study an enhanced local approach model developed by Hohe et al. [11] considering the maximum principal stress $\sigma_1$, the accumulated equivalent plastic strain $\varepsilon_{eq}^{pl}$, and the local stress triaxiality $h$ as quantities controlling cleavage fracture was used for following numerical assessments. The incrementally formulated version of this model describes the increase in fracture probability of a volume element $dV^{(i)}$ by

$$dp_f^{(i)} = f_{nuc}^{(i)}(\varepsilon_{eq}^{pl}, h) \cdot f_{inst}(\sigma_1)dV^{(i)} \quad (2)$$

as a function of the probability of the evolution of potentially critical microdefects $f_{nuc}^{(i)}(\varepsilon_{eq}^{pl}, h)$ and the probability of instability $f_{inst}(\sigma_1)$. Instability is described by the Griffith-Criterion, and depending on presumed particle size distribution, leads to

$$f_{inst}(\sigma_1) = \begin{cases} \left( \frac{\sigma_1}{\sigma_u} \right)^m - \left( \frac{\sigma_{th}}{\sigma_u} \right)^m \frac{e^{2\left( \frac{\sigma_u}{\sigma_1} \right)^2} - e^{2\left( \frac{\sigma_u}{\sigma_{th}} \right)^2}}{2} \\ \sigma_{th} \frac{e^{2\left( \frac{\sigma_u}{\sigma_1} \right)^2} - e^{2\left( \frac{\sigma_u}{\sigma_{th}} \right)^2}}{2} \end{cases} \quad (3)$$

(top: power distribution, bottom: exponential distribution; $\sigma_{th}$, $\sigma_u$, $m$: parameters).

In this study an exponential particle distribution is assumed. Brittle particle fracture however is only a necessary condition for unstable cleavage fracture. The second condition is the presence of critical microdefects. As mentioned earlier, it was shown in [11] that the nucleation of critical microdefects can be described as a function of the equivalent plastic strain and the stress triaxiality. The mechanism of crack nucleation controlled by plastic strain has previously been considered by models from authors like Faleskog et al. [9] and the influence of stress triaxiality by for example Chen et al. [8]. The evolution term for critical cracks in the enhanced cleavage fracture model was derived from an analysis of local conditions at the origin of cleavage fracture and formulated as

$$f_{nuc}^{(i)}(\varepsilon_{eq}^{pl}, h) = c_2 \cdot e^{-c_1h} \frac{d\varepsilon_{eq}^{pl} - c_1\varepsilon_{eq}^{pl}}{\sqrt{1+(c_1\varepsilon_{eq}^{pl})^2}} dh \quad (4)$$

with $d\varepsilon_{eq}^{pl} > 0$ and $d\varepsilon_{eq}^{pl} - c_1\varepsilon_{eq}^{pl} dh > 0 \quad (5)$

with the material parameters $c_1$ and $c_2$. Higher probability of microdefect evolution via particle fracture upon increased plastic deformation is regarded in these formulations. The accumulated failure probability $dP_f^{(i)}$ of the volume element $dV^{(i)}$ emerges from the integration of the failure probability increments $dp_f^{(i)}$ until the current point in time. The mentioned weakest-link-concept is applied here as well, and reveals the accumulated failure probability of the overall structure to

$$P_f = 1 - e^{\int_0^{t} dp_f} \quad (6)$$

Ultimately, the model is capable of considering the temperature dependency of cleavage fracture by a temperature dependent nucleation term. It could be shown in [11] that the maximum stress that leads to cleavage initiation is quite independent on the test temperature, therefore the instability term $f_{inst}(\sigma_1)$ can also be assumed as temperature independent. On the other hand, the
plastic strain and the corresponding stress triaxiality are temperature-dependent quantities and also the nucleation of critical microdefects is a temperature dependent effect since at higher temperatures a microdefect could undergo plastic deformation and become uncritical via blunting at the crack tip. Therefore, it seems plausible to describe the temperature dependency of the fracture toughness by a temperature dependent nucleation term as shown in the following paragraph.

Important regarding fracture mechanics assessment under transient thermomechanical loading is also the fact that this incrementally formulated model is suitable to describe the load history due to the fact that it considers directly the existing stresses and strains and current temperatures at the respective location during the individual load paths. Noteworthy also, the instance that according to equation (5) an increasing plastic deformation must be present to increase fracture probability (active plasticity).

### 2.3 Numerical Adjustments

An example for the used finite-element mesh can be seen in Fig. 5. For reasons of numerical stability a crack front with a radius of 15 µm (d = 30 µm) was used for all models (isothermal and transient loading conditions). The software used was ABAQUS, and the fracture mechanics specimens were modelled benefitting from the geometry's symmetry characteristics (one quarter specimen) by fully-integrated 8-node volume elements with a linear displacement function. The crack front is assumed to be straight, and an experimentally determined representative crack length ratio was applied according to the different specimen types. The displacement-controlled loads and anvils were modelled by ridged-body cylinders. The interaction between specimen and rigid bodies was modelled nearly friction-free (μ = 0.001, penalty method). All calculations were conducted geometrically non-linear with consideration of large plastic deformations by using an implicit solver. Regarding elastic-plastic material properties and for reasons of numerical stability, the Luders Band was approximated with a slight incline of 5 MPa, overlapping of the curves in this region was impeded, and the curves were extrapolated linearly at higher strains to ε = 5 where data was non-existent. The elastic material properties were described by Hooke’s law with a temperature-dependent Young’s modulus, and the plastic behavior by the v. Mises flow model with isotropic hardening. In addition, a temperature-dependent thermal expansion coefficient was implemented.

The \( J \)-Integral at the crack tip was calculated by ABAQUS contour integrals and weighted according to the respective element size along the crack tip, after which an effective \( J \)-Integral \( J_{\text{eff}} \) was obtained that represents the entire crack front, and used to calculate the relevant load \( K_J \) with the expression

\[
K_J = \frac{J_{\text{eff}} E(T)}{\sqrt{(1-\nu^2)}}
\]

\( (E: \text{temperature-dependent Young's Modulus}; \nu: \text{Poisson's Ratio}). \)
The model's parameters are the constraint parameter $c_1$, the threshold stress $\sigma_{th}$, a scale parameter $\sigma_u$, and the proportionality factor $c_2$. The parameter $m$ is not used in this study, because it is only used for a power distribution of the particles, while here an exponential distribution is assumed (see equation (3)). According to Hohe et al. [11], due to the mathematical formulation of the model, one of the parameters $\sigma_u$, $\sigma_{th}$ is surplus so that $\sigma_u$ could be set to a fixed value. Petti et al. [22] propose a temperature-dependency of $\sigma_u$, linked to local events that include plastic shielding of microdefects or microdefect blunting. However, this does not contradict the procedure in this study due to the fact that the used model in [22] only considers the instability of microdefects in terms of the original Beremin model [5], and does not consider microdefect evolution or blunting like the model proposed by Hohe et al. [11].

The parameter $\sigma_u$ is necessary for reasons of dimension in this model formulation, and can be combined with $c_2$ (which is adjusted), therefore having no individual effect contrary to the original Beremin model for example. In this model $\sigma_u$ is interpreted as a model parameter with a physical background. It is derived from the Griffith criteria regarding the largest possible microdefect, or rather its corresponding stress leading to instability. Since lower stress is needed for the instability of larger microdefects, yet the size of microdefects is limited in reality, $\sigma_u$ is considered a threshold-stress beneath which cleavage fracture does not originate. This lower boundary is considered similar to the parameter $K_{min}$ in the Master Curve concept. A parameter study in [11] showed that an increase in $\sigma_u$ leads to less scatter in the calculated probability of failure, which indeed showed slightly better results compared to the experimental data. However, since an analysis of the maximum principal stress during the development of the model showed that cleavage initiation generally occurs between 1400 and 1900 MPa, a choice of higher $\sigma_u$ values is not favorable with regards to the physical meaning of $\sigma_{th}$, and good results with the adjustment of the other parameters instead were achievable as well.

The parameter $c_1$ scales the influence of the local constraint conditions in the defect nucleation term. A change of the value $c_1$, therefore impacts the calculated failure probability differently depending on specimen geometry, or actual constraint condition at the crack tip. According to [10] a reduction of $c_1 = 1.5$ (which is considered a good fit to this material) causes a general increase in probability of failure for high constraint conditions, while the impact is only very slight for low constraint conditions such as shallow-cracked specimens.
So conclusively, the following parameter configuration was derived suitable for the examined material: \( c_1 = 1.5; \sigma_m = 1400 \) MPa; \( \sigma_u = 1400 \) MPa. For this rather practical approach the intention was to adjust solely the parameter \( c_2 \) to the temperature as described in the previous chapter. It can be seen as a proportionality constant for a term that describes the materials potential to nucleate a critical crack. Because it also respects the influence of stress triaxiality \( h \), the parameter does not only account for crack nucleation in general linked to plastic deformation, but also its potential to remain sharp and not blunt (criticality). This was identified to be temperature-dependent. Therefore, lower values of \( c_2 \) for the critical nucleation term are associated with higher temperatures because blunting here is common (see Fig. 6 right). Lower temperatures impede this mechanism resulting in higher \( c_2 \)-values. Moreover, the decline of \( c_2 \) below -135 °C is linked to the inaccuracy of the Master Curve (further discussed below).

The experimentally extracted \( T_{0,C(T)} \) under isothermal conditions can be used to reconstruct the probability of failure based on the Master Curve concept as a function of load \( (K_J) \) for individual temperatures (colored lines), Fig. 6 left. Subsequently, these isothermal tests are simulated, and the local approach model (parameter \( c_2 \)) is adjusted by the method of least squares so that failure probability predicted by the local approach model matches the assessment of the Master Curve. A model parameter adjustment is therefore conducted solely with the knowledge of the \( T_0 \)-reference temperature. The result is a temperature dependency of the material parameter \( c_2 \), Fig. 6 right. This adjustment was only applied to C(T) specimens, but used for all numerical assessments.

Fig. 6 left shows in general a good match of the isothermal Master Curve for the experimental \( T_{0,C(T)} \) (colored lines) with the model (dashed lines). This agreement is excellent for temperatures around \( T_{0,C(T)} = -91 \) °C, yet slightly declines towards very low temperatures below -135 °C (brown line). Due to the parameter fitting procedure using the least square method the model matches the 50% failure probability for the low temperatures quite well leading to an unexpected decline in \( c_2(T) \) as shown in Fig. 6 right. In contrast to the mean value the distribution functions at these low temperatures result in some deviations from the Weibull distribution of the Master Curve. This issue will be further discussed in chapter 4.

![Fig. 6: Accumulated probability of failure as a function of load for isothermal conditions by Master Curve (colored lines) and the adjustment of the model under these isothermal conditions (black dashed lines). The parameter \( c_2 \) is adjusted to the Master Curve of the material under isothermal conditions. The result is a temperature dependency of the material parameter which is implemented into the model.](image)
3 Results

The experimental and numerical results are shown in Fig. 7 - Fig. 10 in the same manner. The solid lines (arrows) represent the individual load paths $K_J(T)$ of the experiments that are recalculated with an average slope of all tests with the same nominal slope starting at the preload at 25 °C. The icons along the pathways show the individual fracture points of the experiments during the load history which could deviate slightly from the average slope. The Master Curve (grey) is also linked to this primary y-axis, and is derived from the isothermal material behavior as a reference. Information regarding the colored dashed lines is connected to the secondary y-axis (right) and shows the accumulated failure probability calculated by the local approach model at a specific period during the individual loading histories. For example, Fig. 7 shows distinctively where the 5 or 50 % failure probabilities are located along the individual load paths, at which temperature the dashed lines predict this specific failure probability. And furthermore, it can be seen that the predicted failure probability at pre-loading at 25 °C is nearly 0 % in all cases. This display method also allows the quick perception of a violation of the Master Curve (isothermal conditions) when the Master Curve does not envelop the individual fracture points with its 5 and 95 % boundaries.

The experimental and numerical results of the influence of varying $dK_JdT$-slopes compared to the isothermal Master Curve are shown in Fig. 7. Starting from the pre-load of $K_J = 165 \text{ MPa} \sqrt{\text{m}}$ a significant increase of fracture toughness can be observed by following a transient load path. Even for the steepest slope of $-0.75 \text{ MPa} \sqrt{\text{m/°C}}$ the majority of specimens fractured beyond the 95 % Master Curve fractile. The benefit in fracture toughness becomes more pronounced for shallower slopes, whereas the shallowest slope (green) even results in non-fractured specimens (grey fracture points). The Master Curve concept in this case represents a very strong conservatism for transient loading situations. 5 % failure probability of the local approach assessment is specifically addressed here due to the fact that it constitutes the lower boundary in the Master Curve concept, as well as 50 % for reasons of further model accuracy.

The model’s fracture probability prediction by numerical assessment considering steep slopes is excellent. The assessment for load path 1 and 2 – considering 5 and 50 % fracture probability – are in complete accordance with the experimental results and slightly conservative. Path 3 shows compliance considering the 5 % fractile, and a more profound conservative evaluation of 50 % failure. The probability distribution below -100 °C for path 3 is described quite satisfyingly, yet the 95 % fractile slightly mismatches the experimental results in a non-conservative manner, after which fracture probability stagnates at around 90 %. Path 4 shows least conformity, resulting in an even more profound conservative calculation of the 5 % fractile. As with very low temperatures of T < -125 °C for path 3, the fracture probability for path 4 moderately and non-conservatively mismatches the experimental data. However, considering that 38 % of the specimens did not experimentally fracture, and a corresponding numerical stagnation of fracture probability is around 48 %, still presents quite good results. Furthermore, the model appears to predict a deviation in fracture probability for very low temperatures of < -100 °C resulting in underestimated fracture probabilities in terms of numerical assessment for very high probabilities of failure (especially cases 3 and 4). Further numerical analysis showed that these changes in slope of $P_f$ are related to the sudden and steeper incline of the yield stress and the complete flow curves at lower temperatures. In terms of the model, this affects two things: the change in plastic deformation $d\varepsilon_p$, and the change in highly-stressed volume. This topic will be addressed in more detail in chapter 4.
Fig. 7: Load paths with individual fracture points (solid lines and icons), and numerical results (accumulated failure probability, dashed lines) regarding the influence of varying $dK/dT$-slopes on fracture toughness of C(T) specimens compared to the isothermal Master Curve.

The influence of a change of pre-load for transient load paths with similar slopes can be observed in Fig. 8. A lower pre-load of 105 MPa$\sqrt{\text{m}}$ causes a significant benefit in fracture toughness compared to the Master Curve under isothermal conditions whereas none of the C(T) specimens fractured before the 95 % fractile. An increase of pre-load to 165 MPa$\sqrt{\text{m}}$ leads to fracture at similar temperatures, but much higher loads. Considering numerical assessment, the entire probability distribution for the low pre-load load path is calculated quite precisely, being slightly conservative for the 5 and 50 % fractiles, while the agreement of experiment and simulation is very good even for the 95 % fractile. Again, the strong conservatism of the Master Curve concept for transient loading situations was proven.
Finally, the influence of various stress conditions (constraint effect) at the crack tip was analyzed by comparing the results of C(T) specimens to SE(B) specimens with similar crack depth ratios of $a_0/W = 0.5$, and also SE(B) specimens with shallow cracks of $a_0/W = 0.13$. Noteworthy here: the parameter adjustment was not re-done for the bending specimens. A change in specimen geometry for $a_0/W = 0.5$ results in dissimilar stress distributions in the vicinity of the crack tip (stress triaxiality $h$). This in terms of cleavage fracture more favorable stress state causes the material to fail at higher load, not only under isothermal conditions, but also under transient loading situations, Fig. 9. Similar to all previously presented results, the 5 % fractile of the SE(B) specimens is also assessed slightly conservatively. 50 % failure probability is calculated over-conservatively and the model accuracy declines strongly below -120 °C. Similar to previously seen observations at very low temperatures, a stagnation of failure probability is calculated numerically yet not witnessed experimentally. In addition, Fig. 9 also shows the temperature shift of the isothermal Master Curve 5 % fractiles (lower bound) due to transient loading according to the numerical assessment by local approach. The benefit in fracture toughness of $\Delta T_{0,LA,C(T)} = -36$ °C and $\Delta T_{0,LA,SE(B)} = -37$ °C compared to the respective isothermal Master Curves due to transient loading is very similar for both specimen types. This allows the conclusion that the WPS-effect has the same impact on fracture toughness for these two different constraint conditions.
Fig. 9: Load paths with individual fracture points (solid lines and icons), and numerical results (accumulated failure probability, dashed lines) regarding the influence of a specimen geometry / stress state for similar crack length ratios of 0.5 for transient load paths with similar slopes.

Fig. 10 depicts the influence of shallower cracks regarding SE(B) specimens for transient loading situations compared to the already discussed SE(B) specimens with $a_0/W = 0.5$, and the isothermal fracture mechanics tests. Following a similar load path, the shallow-crack specimens generally do not fracture before -109 °C, whereas the first fracture of the specimens with $a_0/W = 0.5$ can experience fracture already at -86 °C. This tendency is not profound, however, it matches the experimental results from the isothermal tests, where a minor influence of crack length was witnessed at higher temperatures of -90 °C. Contrary to this, but similar to the isothermal test as well, there appears to be only a very minor difference in the benefit of fracture toughness – if any at all - due to transient loading in favor of the shallow-crack specimens at lower temperatures of < -110 °C. This strengthens the mentioned theory that a loss of constraint is not relevant at very low temperatures.

Furthermore, as stated in chapter 2.1, due to the relatively tough ground state of the material, and very low testing temperatures, the isothermal Master Curve for SE(B) specimens with $a_0/W = 0.13$ presumably does not quantify the constraint-effect adequately, hence the relevance of the depicted 5% Master Curve fractile, as well as the shown shift of $\Delta T_{0,LA,SE(B)a/W=0.13} = -72$ °C, is questionable. A more realistic isothermal Master Curve reference temperature $T_0$ for SE(B) specimens with $a_0/W = 0.13$ of roughly 20 °C lower than $T_{0,SE(B)iso,a/W=0.13} = -115$ °C (as reported by Hohe et al. [12]) would cause more similar benefits of $\Delta T_{0,LA} \approx -50$ °C like seen in Fig. 9.

Considering the quality of numerical assessment for shallow-crack SE(B) specimens, it is obvious that even for fundamentally different stress conditions at the crack tip the 5% fractile is calculated quite accurately, yet again with slight conservatism. However, higher failure probabilities of about > 30% are increasingly underestimated, which coincides well with the previous numerical observations.
Fig. 10: Load paths with individual fracture points (solid lines and icons), and numerical results (accumulated failure probability, dashed lines) regarding the influence of a specimen geometry / stress state for deep (0.5) and shallow cracks (0,13) for transient load paths with similar slopes.

Fig. 11 shows an exemplary transient load path with the calculated failure probability by local approach (red), and the isothermal Master Curve 5 % boundary (black). While following the load path it is evident that the isothermal Master Curve 5 % boundary is over-conservative, and the local approach provides a very accurate prediction. However, a great advantage of the Master Curve concept is that differences in fracture toughness can be expressed conveniently by a $T_0$-shift. With this in mind, it seems reasonable to construct a new Master Curve $MC_{LA}$ with the probability of failure of 5 % (chosen due to the acceptance of it as a lower boundary) matching the predictions of the local approach (blue) regarding the individual load paths. Now, a $\Delta T_{0,LA,5\%}$ can be derived as a benefit in fracture toughness, keeping in mind that under isothermal conditions the $T_0$-shift of all percent-fractiles is identical. Conclusively, the benefits in fracture toughness through transient loading, represented by these $\Delta T_{0,LA,5\%}$ can be examined as a function of the slope $dK_J/dT$. This is displayed in Fig. 12, yet the slope $dK_J/dT$ was replaced by the geometric angle of the slope, due to fact that isothermal conditions take place at $dK_J/dT \to \infty$, which for obvious reasons is impractical for displaying. It is noteworthy here that the geometric angle was calculated based on similar unit lengths in the diagram (1 MPa/$\sqrt{m}$ ↔ 1 °C), and not according to the arbitrary relation in for example Fig. 7. Fig. 12 ranges from isothermal conditions with 90° and the highest fracture probability (covered by the Master Curve $\Delta T_{0,MC}$) to the load cool fracture transient with 0° and no fracture ($\Delta T_0 \to -\infty$). The extrapolated courses of $\Delta T_{0,LA,5\%}$ (dashed lines) neatly match these experimentally proven observations, and further highlight the applicability of this assessment method. Also, Fig. 12 again shows the great conservatism of the Master Curve which becomes stronger with decreasing slope/angle, because it always predicts a benefit of $\Delta T_0 = 0$ °C. Moreover, the figure also features $\Delta T_0$-values of Master Curves derived from the individual experimental fracture points of the load transients,
meaning simply an application of the Master Curve formalism with these fracture points according to ASTM E1921 [4]. The distribution functions associated with this “Transient” Master Curve method are not validated, but in this case the method is used solely as a tool to average the experimental results due to its easy applicability. This resulting “transient” Master Curve $\Delta T_0$ in Fig. 12 is not necessarily conservative, yet can be used as a rough and simple estimation of the safety margin due to transient loading. However, a more precise and slightly conservative assessment of the failure probability under transient loading could be achieved with the local approach model.

**Fig. 11:** Example of a “corresponding” Master Curve (blue) that shows the same probability of failure of 5% where the local approach model predicts it. This allows the quantification of a benefit in fracture toughness through $\Delta T_{0,LA}$.

**Fig. 12:** Benefit in fracture toughness (represented by $\Delta T_0$) as a function of the angle of the slope in the range of isothermal testing conditions (90 ° with no benefit) to horizontal load cool fracture transients (0 °C with no fracture). $\Delta T_0$ of the “Transient” Master Curve represents an averaging method of the experiments.
4 Discussion

In general, and considering practical relevance in safety assessment, the advanced cleavage fracture model is able to describe the probability of fracture and the benefit in fracture toughness in an excellent manner. However, for shallower loading paths/lower temperatures of $T < -100 \degree C$ the model generally underestimates fracture probability compared to the experimental results. At this point it should be noted that these low temperatures at fracture cannot be reached in real cases, but the experiments represent the situation for irradiated materials where the reference temperature $T_{0,irr}$ shows a positive value. In such cases the fracture toughness curve, as well as the load paths, are shifted to higher temperatures and the effects are comparable to the investigations presented here.

For all cases investigated the strong over-conservatism (at least $\Delta T_0 = +20 \degree C$) of the Master Curve concept for transient loading situations was demonstrated (considering 5 % failure probability), while the more advanced local approach method was able to lower the conservatism to an acceptable minimum. Even fundamentally different stress conditions at the crack tip are correctly taken into account in terms of their impact on cleavage fracture probability, while model parameters were only adjusted to isothermal simulations containing one geometry type.

The advanced cleavage model was developed for, and based upon, ferritic steels in the transition range, not considering micromechanical effects at very low temperatures in connection with small capacities of plastic deformation. Equation (4) postulates that the microdefect nucleation term becomes smaller with decreasing plastification $d\varepsilon_{pl}$. Plastification strongly decreases with temperature reduction due to the climb of flow stress within the material. Consequently, the probability of particle fracture due to plastic matrix deformation is reduced and the growth in fracture probability declines as well. Very low temperatures however ($T < -100 \degree C$) cause higher stresses of $>2000$ MPa that are not easily relieved by plasticity, and can cause particles to fracture by dislocation pile-up or direct fracture because of these high stresses. These mechanisms gain importance with decreasing temperature, which corresponds to the increasing underestimation of fracture probability with decreasing temperature.

Particularly graphs 3 and 4 in Fig. 7 revealed sudden points of discontinuity regarding the prediction of failure probability for lower temperatures. The change in plastic deformation $d\varepsilon_{pl}$, and the change in highly-stressed volume were mentioned as relevant here in terms of the model. The sudden and steeper incline at lower temperatures in yield stress at the grid points of the flow curves (-100, -120, -135, -150 °C) cause a point of discontinuity, since nucleation probability in equation (4) depends directly on the change in plastic deformation $d\varepsilon_{pl}$. Only volume elements which witness an ongoing incremental change in plastic deformation $d\varepsilon_{pl} > 0$ are considered for cleavage initiation (highly-stressed volume). In relative terms, this reduction in highly-stressed volume due to the temperature dependency of the flow curve is stronger for shallower $dK/dT$ slopes, because steeper slopes naturally have a stronger increase in load. It seems plausible that the description of very low changes in plastic deformation with this material law constitutes one reason for the experimental discrepancies at very low temperatures, yet similar problems were observed for very steep $dK/dT$ slopes with SE(B) specimens that fracture at lower temperatures due to their loss of constraint.

An additional explanation for the discrepancies at lower temperatures is that the numerical calculation was based on the shape of the Master Curve which is not supported by isothermal tests at these low temperatures. Furthermore it can be seen from Fig. 6 a) that even for isothermal loading the distribution function of the failure probability is not matched with the numerical model. To improve the model accuracy for very low temperatures, additional isothermal tests at low temperatures would be necessary as well as extensions of the model for cleavage failure in the lower shelf region.
A change of the model parameters without any additional tests at low temperatures were proven as not constructive to resolve the mentioned discrepancies. A higher threshold-stress parameter $\sigma_{th}$ for instance would only result in less scatter of failure probability, whereas the physical background of the parameter would be ignored as well. As already discussed in the numerical adjustments 2.3, a reduction of the constraint parameter $c_1$ would only have very little effect on the shallow-cracked specimens with low constraint conditions, whereas an adjustment of the C(T) specimens with $a_0/W = 0.5$ is not necessary because of the excellent results.

Concerning the constraint effect, Fig. 9 shows that the benefit in fracture toughness due to transient loading or the WPS-effect is very similar for C(T) and SE(B) specimens, or more specifically, their stress states at the vicinity of the crack tip. Most likely, this is also the case regarding a reduction of crack length, yet it is not certain. The model inaccuracies for SE(B) specimens considering higher probabilities of failure are most likely linked to the corresponding lower temperatures that are not relevant for C(T) specimens with this slope.

The model's limited applicability for very low temperatures of $<-120$ °C however, is strongest for shallow-crack SE(B) specimens. The much stronger underestimation of higher fracture probabilities here cannot only be interpreted by the mentioned explanation attempts, because similar temperatures are also reached by other specimen types. In particular, higher relevance of crack arrest has been reported under isothermal testing conditions for shallow-crack SE(B) specimens by Hohe et al. [12]. Due to the strong loss of constraint, increased plastic zones are created during loading which could promote arrest. Influences such as multiple cleavage initiation sites are imaginable as well at these very low temperatures, yet a concrete physical explanation remains absent. However, it is to be stressed again that the relevance of this limited applicability is only based on scientific motivation.

Moreover, due to the model's good assessment qualities for SE(B) specimens of different crack lengths by using a previous parameter adjustment to C(T) specimens, the physical foundation of the model is further reassured because the parameters appear to have a micromechanical meaning.

The previously unknown limitations of the model (discrepancies at very low temperatures) constitute no immediate problem in terms of practical safety assessment, and are rather of scientific relevance. However, already mentioned examinations concerning irradiated materials could be of practical interest as well, not only to experimentally classify fracture behavior, but to also assess it numerically.

5 Conclusions

The objective of this study was to investigate the influence of slope, pre-load, and specimen type (stress condition) on the fracture behavior of a ferritic-bainitic pressure vessel steel under transient thermomechanical loading situations. In all cases a strong benefit in fracture toughness was observed compared to isothermal testing conditions. The benefit increases systematically with shallower slopes and larger pre-stresses. Transient loading paths for different crack and specimen geometries (or stress conditions at the crack-tip) lead to very similar benefits in fracture toughness compared to their isothermal reference states.

All experimental load paths were numerically assessed by using an appropriate incrementally formulated local approach model, and for all cases the 5% fracture probabilities (as a lower boundary) were calculated in a slightly conservative manner. The strong over-conservatism of the Master Curve concept for transient load paths was demonstrated, and it can be reduced to a reasonable minimum by the usage of local approach. In addition, most 50%, and even some
95% fracture probabilities, were also calculated accurately and slightly conservatively. Nevertheless, previously unknown limitations of the model were revealed regarding very low temperatures, which then again are irrelevant for these types of emergency cooling scenarios.

The simple parameter adjustment of C(T) specimens to the isothermal Master Curve of the material performs well, especially considering the good results after using these parameters for the assessment of SE(B) specimens with varying crack lengths.

Acknowledgement

The investigations were supported by the Federal Ministry for Economic Affairs and Energy under the support code 1501439 which is thankfully acknowledged by the authors.

References


Petti, J.R., Dodds, R.H.: Calibration of the Weibull stress scale parameter using the master curve, Engineering Fracture Mechanics 72 (2005) 91-120.


