On the identification and uniqueness of constitutive parameters for a non-local GTN-model

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The present study proposes a parameter identification and calibration strategy for a specific non-local GTN-model, which has been developed to circumvent spurious mesh dependency during simulation of ductile failure. The parameter calibration strategy is applied to an experimental database of a pressure vessel steel tested at moderate to high stress triaxialities. Relevant parameters of the non-local GTN-model can be identified using simulated/experimental crack growth resistance curves determined by a fracture mechanics test (Mode I loading). In addition, only results of a smooth tensile test are utilized in order to identify an appropriate strain hardening law. Based on this input information, the failure behavior of smooth and notched tensile specimens as well as miniaturized deep drawing tests is predicted by finite element simulations. A fairly good agreement with experiments is obtained, which validates the feasibility of the suggested approach.

Keywords: reactor pressure vessel steel 18Cr2MFA; gradient-enhanced damage modeling; ductile damage; gradient-enhanced damage; calibration strategy; finite element implementation; ductile failure; application

1. Introduction

Ductile damage is microscopically characterized by nucleation, growth, and coalescence of microvoids. Motivated by the void growth mechanism, Gurson [1] developed a micromechanically based pressure dependent plasticity model, which can be used to predict material softening. Further improvements by Tvergaard and Needleman [2, 3, 4] established the so-called Gurson-Tvergaard-Needleman model (GTN) as highly accepted tool within the local approaches to fracture. Nowadays, the model is implemented by default in commercial FEM-codes to analyze engineering problems. However, the original GTN-model exhibits spurious mesh dependency.

In order to circumvent the pathological mesh dependency due to ill-posedness of the underlying boundary value problem, several heuristic regularization methods are proposed. These regularized variants of the GTN-model are called non-local models in the following. For example, non-local spatial averaging [3, 6, 7] as well as gradient-enhancements [8, 9, 10, 11] are suggested. Non-local damage variables [6, 8, 9] or non-local driving forces of void evolution [10, 11] are investigated. The common gradient-enhanced models involve an additional field equation, which contains the chosen non-local variable as degree of freedom. This PDE of Helmholtz-type is well known from implicit gradient-enhancement suggested by Peerlings et al. [12], which can be directly deduced from non-local spatial averaging.
Alternatively, gradient extensions of Gurson’s model are deduced, which are based on sound homogenization frameworks, e.g., the micro-dilatational approach of Hütter [13] and the strain gradient extension of Gologanu et al. [14] (GLPD-model). As a result, higher order stresses enter the yield function in case of both models and numerically treatment can become sophisticated. In contrast, heuristic implicit gradient extensions which only utilize a scalar non-local variable can be efficiently implemented into commercial FE-software as demonstrated by Seupel et al. [15] and Azinpour et al. [16]. Therefore, the model of Linse et al. [10] is the starting point of the present paper, which is based on a gradient-enhanced volumetric plastic strain motivated by micro-dilatational theory. In addition to the common model parameters of the local GTN-model, a length parameter \( l_{nl} \) occurs in the gradient-enhanced approach.

The suggested model has already been applied to simulate ductile failure of a pressure vessel steel during small punch testing [17]. Therein and in other studies [18, 19, 9], assumptions concerning the internal length are made rather than performing a proper identification and calibration. Moreover, practicable parameter identification strategies for non-local models are barely discussed, excepting [20, 21, 11].

On the basis of principal investigations on ductile crack initiation and propagation, Hütter et al. [20] deduced a possible method to determine the damage related parameters for the considered non-local GTN-model. Fracture mechanics tests providing stable crack growth data can be used to separate the influence of the model parameters.

In the present paper, the calibration strategy for the non-local GTN-model proposed by Hütter et al. [20] is assessed using an experimental database of the pressure vessel steel 18Ch2MFA (comparable to 17CrMoV 9 [22]). Results on a fracture mechanics test, smooth and notched tensile tests as well as a miniaturized deep drawing test (Small Punch Test—SPT) are available from literature [23, 24, 25, 21]. Moderate to high stress triaxialities occur in the critical regions of the testing specimens [21]. Therefore, modifications of the GTN-model concerning shear loading cases need not to be included at the moment, see [26]. As calibration basis, results of the smooth tensile test and the crack growth resistance curve from fracture mechanics test are used, which are typically accessible for similar materials with regard to further engineering applications of the model. Using the identified parameter sets, notched tensile tests and the small punch test are simulated in order to evaluate the validity of the considered approach and to work out some suggestions for proper application.

The paper is organized as follows: In section two, the material model and its gradient-enhancement are briefly recapitulated including some slight modifications with respect to the original setup of Linse et al. [10]. An efficient implementation into the commercial FE-code ABAQUS [27] is proposed using the similarity of the additional balance equation of Helmholzt-type for the non-local variable and the well known steady state heat equation as suggested and implemented in [15, 16, 28]. In the third section, material characterization, experimental results, and the FE-models of testing setups are summarized. Section 4 starts with a careful sensitivity study to investigate the influence of the damage parameters for the different types of tests. Afterwards, the model calibration is conducted according to the developed strategy and the model validity is evaluated. Finally, recommendations are provided on how to choose the model parameters with respect to accuracy of predictions and computational efficiency.

2. Non-local GTN-model

2.1. Constitutive equations

The constitutive equations of the GTN-model are introduced using hypoelasticity to account for finite deformations. The objective Jaumann-rate of stress is utilized, which enables a direct implementation into the FE-code ABAQUS via its user material interface UMAT. For simulations of typical industrial forming processes, Brepols et al. [29] figured out that predictions of proper hyperelastic based plasticity models, consistent rate formulations, and the hypoelastic approach exhibit nearly the same results.
Therefore, and for reasons of simplicity, the hypoelastic basis should be tolerated.

The hypoelastic stress-strain relation is based on the assumption of splitting the deformation rate \( \dot{D} \) into an elastic and a plastic part, \( D_{el} \) and \( D_{pl} \), respectively:

\[
\sigma^\prime = C : D_{el}, \quad D_{el} = D - D_{pl}. \tag{1}
\]

Therein, \( \sigma^\prime \) and \( C \) denote the objective Jaumann-rate of the Cauchy-stress tensor \( \sigma \) and the isotropic elasticity tensor of order four, respectively.

Following the GTN-approach, the yield function and loading/unloading conditions of rate independent, pressure influenced plasticity read

\[
\Phi = \frac{\sigma_y^2}{\sigma_y^2} + 2q_1 f^* \cosh \left( \frac{3q_2 \sigma_h}{2\sigma_y} \right) - \left( 1 + (q_1 f^*)^2 \right) \leq 0, \quad \Lambda_{pl} \geq 0, \quad \Lambda_{pl} \Phi = 0, \tag{2}
\]

with the plastic multiplier \( \Lambda_{pl} \) and the empirical model parameters \( q_1, q_2 \). The equivalent stress \( \sigma_{eq} \) and the hydrostatic stress \( \sigma_h \) are extracted from the stress tensor and the stress deviator \( S \), respectively:

\[
\sigma_h = \frac{1}{3} \text{tr} (\sigma), \quad S = \sigma - \sigma_h \delta, \quad \sigma_{eq} = \sqrt{\frac{3}{2} S : S}. \tag{3}
\]

The unity tensor of second order is denoted as \( \delta \). Material softening is obtained through the evolution of porosity \( f \) entering the yield function by its effective counterpart \( f^* \), which is defined in the subsequent section. The yield function shrinks with increasing \( f^* \). At \( f^* = 1/q_1 \), the load carrying capacity vanishes.

Associated plasticity is assumed, which defines the plastic rate of deformation as

\[
D_{pl} = \Lambda_{pl} \frac{\partial \Phi}{\partial \sigma} = \dot{\varepsilon}_{eq} N + \dot{\varepsilon}_h \delta, \quad N = \frac{3}{2\sigma_{eq}} S. \tag{4}
\]

For convenience, the rates of equivalent plastic strain \( \dot{\varepsilon}_{eq} \) and volumetric plastic strain \( \dot{\varepsilon}_h \) are introduced:

\[
\dot{\varepsilon}_{eq} = \Lambda_{pl} \frac{\partial \Phi}{\partial \sigma_{eq}} = \Lambda_{pl} 2\sigma_{eq} \sigma_y^2, \quad \dot{\varepsilon}_h = \Lambda_{pl} \frac{1}{3} \frac{\partial \Phi}{\partial \sigma_h} = \Lambda_{pl} \frac{q_1 q_2 f^*}{\sigma_y} \sinh \left( \frac{3q_2 \sigma_h}{2\sigma_y} \right). \tag{5}
\]

Isotropic strain hardening can be prescribed by the yield stress \( \sigma_y \) depending on the evolution of the hardening variable \( r \). The rate of hardening \( \dot{r} \) is deduced from the power equivalence between macroscopic quantities \( (\sigma : D_{pl}) \) and the volume preserving matrix material \((\sigma_y \dot{r})\) :

\[
\sigma_y (r) \dot{r} (1 - f) = \sigma : D_{pl} \quad \Rightarrow \quad \dot{r} = \frac{\sigma_{eq} \dot{\varepsilon}_{eq} + 3\sigma_h \dot{\varepsilon}_h}{(1 - f) \sigma_y (r)}. \tag{6}
\]

In case of vanishing porosity, the hardening variable \( r \) coincides with the equivalent plastic strain \( \varepsilon_{eq} \).

### 2.2. Implicit gradient-enhancement

Following the implicit gradient approach of Peerlings et al. \[12\], the mechanical boundary value problem is extended by a Helmholtz-type equation for the non-local variable. According to Linse et al. \[10\], a non-local counterpart \( \xi_h \) of the scalar-valued volumetric plastic strain \( \varepsilon_h \) is defined. Because of the considered direct dependence of void volume fraction on non-local volumetric plastic strain, a regularization of the underlying boundary value problem is attained. As shown with help of a stability analysis in \[10\], the boundary value problem will be unconditionally well-posed if void growth is considered as softening mechanism and void nucleation is neglected.

The additional balance equation of Helmholtz-type reads

\[
\frac{\partial^2}{\partial r^2} \Delta \xi_h = \varepsilon_h - \varepsilon_h \quad \forall \vec{r} \in \Omega \tag{7}
\]
considering trivial Neumann-boundary conditions

\[ \text{grad}_x \tilde{\varepsilon}_h \cdot \vec{n} = 0 \quad \forall \vec{r} \in \partial \Omega, \tag{8} \]

which are justified elsewhere [12, 20]. In Eq. (7), the internal length \( l_{nl} \) occurs as model parameter to be determined. The spatial Laplacian-operator, the boundary’s normal vector, and the spatial gradient operator are denoted as \( \Delta_x \), \( \vec{n} \), and \( \text{grad}_x \) respectively.

The mechanical boundary value problem for the static case is completed by the mechanical balances (static equilibrium condition, moment of momentum)

\[ \text{div}_x \sigma = 0, \quad \sigma = \sigma^T, \quad \forall \vec{r} \in \Omega, \tag{9} \]

and appropriate boundary conditions.

The evolution of \( f \) is directly related to the change in volume \( \dot{\varepsilon}_h \) assuming an incompressible matrix behavior. The regularization of the boundary value problem is attained by relating the void growth \( \dot{f} \) to the evolution of the non-local volumetric plastic strain \( \dot{\varepsilon}_h \):

\[ \dot{f} = 3 (1 - f) \dot{\kappa}. \tag{10} \]

Note that the auxiliary variable \( \kappa \) contains the non-local volumetric plastic strain by introducing the additional conditions

\[ \dot{\kappa} \geq 0, \quad \dot{\kappa} (\dot{\varepsilon}_h - \kappa) = 0, \quad \dot{\varepsilon}_h - \kappa \leq 0, \tag{11} \]

as suggested in [30], i.e., \( \kappa \) corresponds to the maximum of \( \dot{\varepsilon}_h \) over all times \( t \) at each material point. This additional restriction is necessary to ensure the damage condition \( \dot{f} \geq 0 \), especially in cases where re-meshing techniques [30, 19] or element deletion [15] are applied.

The accelerated void evolution, which is considered by the effective porosity \( f^* \) within the GTN-framework, is slightly modified in the present paper:

\[ f^*(f) = \begin{cases} f & f \leq f_c \\ f_c + k (f - f_c) & f_c < f \leq f_u \\ f_u \left(1 - \exp \left(-a_t (f - b_t)\right)\right) & f_u < f \end{cases} \tag{12} \]

After exceeding the critical value \( f_c \), the accelerated void evolution is controlled by the parameter \( k \geq 1 \). Material failure is theoretically reached at the effective porosity \( f^* = f_t^* = 1/q_t \). To ensure a robust numerical treatment of total material damage, Seupel and Kuna [31] propose a continuous and continuously differentiable transition to a nearly failure state, which automatically ensures \( f^* < f_t^* \) and \( f^* \geq 0 \) during numerical solution. This is realized by the third case in Eq. (12). The numerical value of final effective porosity is set to \( f_u^* = 0.995 f_t^* \) throughout the study. The transition value from linear acceleration to saturation is prescribed as \( f_u^* = 0.98 f_t^* \). The transition value of the effective porosity \( f_u^* \) corresponds to a transition value \( f_u \) of the "real" porosity \( f \), \( f_u = (f_u^* + f_c (k - 1))/k \), which is used in Eq. (12). At \( f_u^* \), the material is considered as totally damaged. The parameters \( a_t \) and \( b_t \) in Eq. (12) are fixed by demanding a continuous and continuously differentiable transition with respect to the variable \( f \):

\[ a_t = \frac{1}{1 - \frac{f_u^*}{f_{max}}}, \quad b_t = f_u^* + \frac{1}{a_t} \ln \left(1 - \frac{f_u^*}{f_{max}}\right). \tag{13} \]

If total failure is encountered, the local source \( \varepsilon_{kh} \) in the Helmholtz-equation (7) is fixed in order to circumvent pathological widening of the totally damaged zone observed in simulations conducted in [32]. This is clearly a patch solution, as mentioned in literature [10, 20, 21]. Advanced methods are
Table 1: Chemical composition of 18Ch2MFA (in mass-%, see [23]).

<table>
<thead>
<tr>
<th></th>
<th>Fe</th>
<th>C</th>
<th>Si</th>
<th>Mn</th>
<th>P</th>
<th>S</th>
<th>Cr</th>
<th>Mo</th>
<th>Ni</th>
<th>V</th>
</tr>
</thead>
<tbody>
<tr>
<td>bal.</td>
<td>0.18</td>
<td>0.26</td>
<td>0.4</td>
<td>0.011</td>
<td>0.011</td>
<td>2.45</td>
<td>0.7</td>
<td>0.14</td>
<td>0.27</td>
<td></td>
</tr>
</tbody>
</table>

generally needed to treat the transition from total failure to crack propagation, cf. [20, 32, 18, 15, 33]. However, the deactivation method is used, because it is expected to exhibit an acceptable behavior. For the considered testing setups to be simulated, reasonable damping of the damage widening effect is observed for the related non-local approach of Seupel and Kuna [21].

The implementation into the FE-code ABAQUS is realized as follows: an additional coding of a finite element formulation is bypassed by using the similarity between the Helmholtz-type equation (7) and the steady state heat equation as proposed by Seupel et al. [15] and shown in A. This could be an attractive feature for industrial application. The numerical solution of the model equations is briefly explained in A including the consistent material tangent, which is necessary within the implicit solution scheme of ABAQUS/standard.

3. Materials and methods

3.1. Material characterization

A detailed characterization of the considered steel 18Ch2MFA used in Russian VVER 440 nuclear pressure vessels is given elsewhere [23]. The chemical composition is indicated in Tab. 1 as determined by Müller [23], which is comparable to steel of grade 17CrMoV 9 [22]. The steel exhibits a yield strength \( R_{p0.2} \) of 654 to 680 MPa and an ultimate tensile strength \( R_m \) of approximately 744 to 774 MPa at room temperature (293.15 K). The corresponding elongation \( A \) and cross section reduction \( Z \) at fracture reach about 20% and 70%, respectively. The microstructure is described as bainitic containing grains of an averaged diameter of 125 \( \mu \)m. Elongated manganese sulfides and globular oxidic inclusions are present, which possibly act as initial voids. At room temperature, deep and large dimples are detected at the fracture surfaces of tested specimen indicating a microscopically ductile damage mechanism.

3.2. Experimental setups and FE-models

Thanks to previous studies, the following experimental database is available for the considered steel [24, 23, 21]: Fracture mechanical properties were investigated using single edge notched bend specimen (SENB) under four-point loading [23]. The geometry and the FE-implementation are illustrated in Fig. 1. For the discretization via finite elements, quadrangular elements with quadratic shape functions for the displacement and linear shape functions for the non-local variable \( \bar{\varepsilon}_h \) are applied within all simulations (reduced integration scheme). In 2D plane strain analysis, the corresponding element type in ABAQUS is CPE8RT; for axi-symmetric models CAX8RT. As determined in previous studies [10, 31, 15, 21], the restriction \( b_e \leq 1/4l_n \) on mesh refinement needs to be satisfied in the damage process zone in order to obtain converged results, where \( b_e \) denotes the edge length of regularly shaped quadrangular/cubical finite elements. The refinement \( b_e = 1/4l_n \) is ensured within all upcoming simulations. Experimentally, the crack extension \( \Delta a \) was recorded by partial unloading technique [23]. The J-integral was estimated by the relation given in [34]:

\[
J = \frac{2U}{B_n(W-a_0)} \left(1 - \frac{\Delta a}{2(W-a_0)}\right)
\]

Therein, \( U \), \( B_n \), \( W \), and \( a_0 \) denote the whole area under the load-deflection curve (dimension of energy), the net thickness, the width, and the initial crack length, respectively. The power law fit to the
experim ental data points at room temperature yields [23]

\[
J = 370 \text{ N/mm} \left( \frac{\Delta a}{l_{mm}} + 0.05 \right)^{0.36},
\]

(15)

The J-values from FE-simulations of the SENB test are evaluated in the same manner, i.e., using the simulated force-deflection curve, whereas crack extension is extracted by direct methods, see Sec. 3.3. Details are highlighted in Fig. 1.

In the FE-simulation of the SENB-test, a 2D plane strain model is utilized. A small radius \( r_t \) is applied at the initial crack tip to avoid large element distortion [20], see Fig. 1 b). The applicability of the chosen radius can be checked only a posteriori. Hütter et al. [20] suggest a value within the range (0.07...0.7) \( l_{nl} \). In a previous study on the same material [21], a radius of \( r_t = 0.05 \text{ mm} \) is proposed and shown to be valid for an expected value of the internal length \( l_{nl} \approx 0.1 \text{ mm} \).

Tests of smooth and notched round tensile bars (notch radius \( R \), see Tab. 2) were performed at room temperature [24, 25]. The longitudinal displacement of applied markers and the diameter reduction were measured with the help of a video extensometer. The FE-models of the notched specimens contain the domain between the markers including the notch region as proposed by Seupel and Kuna [21], see Fig 2 a). The smooth tensile tests are modeled including a part of the clamping, which naturally initiates necking in the middle of the specimen due to a small stress concentration, see [21].

Symmetry conditions are utilized for the FE-simulations of tensile and SENB-tests, which is a simplification. In general, cracks can break the symmetry of the problem, e.g., during formation of cup-cone pattern in tensile tests [35]. For the current testing setups the cracks will occur at the symmetry line, but no crack deflection is expected for the simulations utilizing the present non-local, purely void growth driven GTN-model. Zhang et al. [11] show for a related non-local GTN-model that cup-formation during tensile test simulation and crack deflection from the geometric symmetry line of fracture mechanics tests in Mode I loading are unlikely due to the neglected influence of void nucleation, which can trigger such effects.

As validation example, the small punch test is considered. The experimental results are taken from [24, 25]. The testing setup with target values of geometry is sketched in Fig. 2 b). Following Abendroth [25] and Seupel and Kuna [21], the as measured geometry is used within the FE-analysis due to the high impact of geometric deviations on resulting force vs. displacement response. Coulomb friction with
Table 2: Dimensions of notched tensile specimen used in FE-calculations (in mm).

<table>
<thead>
<tr>
<th>label</th>
<th>$R$</th>
<th>$d_0$</th>
<th>$d_1$</th>
<th>$l_0$</th>
</tr>
</thead>
<tbody>
<tr>
<td>RS</td>
<td>$\infty$</td>
<td>5.973</td>
<td>5.973</td>
<td>17.86</td>
</tr>
<tr>
<td>R1</td>
<td>1.04</td>
<td>5.98</td>
<td>11.94</td>
<td>12.78</td>
</tr>
<tr>
<td>R2</td>
<td>1.945</td>
<td>6.205</td>
<td>11.925</td>
<td>13.09</td>
</tr>
<tr>
<td>R4</td>
<td>4.0</td>
<td>6.005</td>
<td>11.935</td>
<td>15.735</td>
</tr>
<tr>
<td>R10</td>
<td>10.075</td>
<td>6.125</td>
<td>11.945</td>
<td>20.515</td>
</tr>
</tbody>
</table>

A constant friction coefficient of 0.25 is chosen between all components according to previous studies [25, 21]. Die, downholder, and punch are modeled as rigid bodies.

3.3. Calibration strategy

For the considered non-local GTN-model, Hütter et al. [20] propose a calibration strategy based on results of a uni-axial tensile test and a fracture mechanics test. Taking into account recent findings [21, 11, 36], the slightly modified procedure reads:

1. Determine the initial porosity $f_0$ from micrographs, chemical composition (Franklin formula for MnS-inclusions) or the like.
2. Choose an appropriate law of isotropic strain hardening using the hardening curve and check by FE-simulation of uni-axial tensile test; neglect damage if $f_0 \leq 0.01$.
3. Calibrate $q_1$ and $q_2$ with help of cell model studies [3, 37, 38] or experiments [11]
4. Choose $f_c$ to fit the tearing modulus of fracture experiments.
5. Adjust $l_{nl}$ to fit fracture initiation toughness.
6. Large-scale yielding: Iterate over points 4-5.

Aiming at a low number of model parameters, the only use of an initial void volume fraction is pursued in the present study, i.e., an additional void nucleation term is omitted. As pointed out by Zhang et al. [11] for a related non-local GTN-model, void nucleation is not necessarily needed to predict ductile failure at moderate to high stress triaxialities as considered here.

4. Results and discussion

In this section, the suggested calibration strategy is discussed in detail. Afterwards, the simulated failure predictions of the smooth/notched tensile tests and the small punch test are incorporated to validate the non-local GTN-model as well as the parameter identification strategy.

4.1. Initial porosity

From the chemical composition for the considered steel given in Tab. 1, an initial void volume fraction $f_0 \approx 5 \cdot 10^{-4}$ is estimated using Franklin’s formula $f_0 = 0.054 (S\% + 0.001Mn\%)$, where chemical constituents are inserted in mass-%. However, Abendroth and Kuna [24] found for the sum of void volume fractions from pre-existing and nucleated pores a value of about 3% during calibration of the local GTN-model. Since we purposely omit a void nucleation term, an $f_0$ higher than $5 \cdot 10^{-4}$ could be justified. Therefore, the applicability of values around the suggested upper bound $f_0 = 0.01$ of Hütter et al. [20] are exploited.
4.2. Strain hardening

Typically, isotropic strain hardening laws for metals in the framework of $J_2$-plasticity are identified with help of the true stress vs. strain curve (hardening curve), which is directly calculated from uni-axial tensile test up to uniform elongation assuming volume preserving behavior. For materials with pronounced necking, as the considered pressure vessel steel, the range of uniform elongation is comparably small, i.e., a good extrapolation of the strain hardening behavior is needed. It is assumed that material softening due to damage can be neglected in the modeling of necking in a considerable deformation range following [36, 21]. Therefore, pure $J_2$-plasticity is used to determine the strain hardening law, i.e., $f_0$ is set to zero. In Fig. 3, the force vs. diameter reduction and force vs. elongation response of the smooth tensile test are plotted for three different hardening laws, which all adequately match the force vs. elongation curve up to the force maximum (uniform elongation). Using a saturating one-term Voce-approach, the response is already underestimated for the considered non-damage case. The power law clearly overestimates the experimental results, which requires a high and sudden influence of damage to achieve a good match beyond uniform elongation. Combining a saturating and a linear term (Voce + linear)

$$
\sigma_y (r) = \sigma_0 + \sigma_{\text{inf}} (1 - \exp (-cr)) + H r
$$

(16)
gives a reasonable prediction of necking for the considered steel as determined by Seupel and Kuna [21], see parameters in Tab. 3.

4.3. Parameters of the GTN-model

Within the subsequent investigations, void growth and material softening become active, i.e., $f_0 > 0$. 

Figure 2: Setups, geometries, and mechanical boundary conditions of a) notched tensile test and b) SPT (target geometry; specimen dimensions: height 0.5 mm, diameter 8 mm). Within FEM-implementation, displacement driven loading $\bar{u}$ is applied. Rotational symmetries are utilized.
Figure 3: Force $F$ vs. a) diameter reduction $-\Delta d/d_0$ and b) elongation $\Delta l/l_0$ response of smooth tensile test RS using different strain hardening approaches for 18Ch2MFA. Pure $J_\infty$-plasticity is assumed. Experimental data from [24, 25].

Table 3: Parameters of the hardening law, equation (16), and elastic properties from [21].

<table>
<thead>
<tr>
<th>Parameter</th>
<th>$\sigma_0$</th>
<th>$H$</th>
<th>$\sigma_{inf}$</th>
<th>$c$</th>
<th>$E$</th>
<th>$\nu$</th>
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<td>MPa</td>
<td>-</td>
<td>MPa</td>
<td>-</td>
</tr>
<tr>
<td>Value</td>
<td>635.485</td>
<td>251.201</td>
<td>156.553</td>
<td>43.463</td>
<td>206500</td>
<td>0.3</td>
</tr>
</tbody>
</table>

The established empirical GTN-parameters $q_1 = 1.5$ and $q_2 = 1.0$ are fixed throughout the study for reasons of simplicity. However, Faleskog et al. [38] show through cell model studies that this set of $q$-parameters is reasonable for steels with moderate strain hardening behavior. An enhanced calibration with help of unit cell models [3, 37, 38] or directly with experiments [11] will be considered in future works.

The parameters $f_c$ and $l_{nl}$ are determined in steps 4-6 of the calibration strategy. The parameter $k$ of the accelerated void growth Eq. (12) is not considered in the proposal of Hütter et al. [20]. Hence, its influence is discussed in what follows. In the present study, just R-curve data is available for a first estimation of the damage parameters. Typically, force vs. load line displacement curves should be considered for more reliable results, too, as performed by Zhang et al. [11]. According to [20], an appropriate set of parameters is expected to be found by performing a relatively simple sensitivity study and a manual adjustment.

A crucial point is the evaluation of crack extension $\Delta a$ to determine the R-curve from simulations. To the authors knowledge, no generally accepted method is proposed in literature. Typical definitions are: averaging of void volume fraction along the ligament [10], position of maximum crack opening stress [20], position of a fixed high porosity value ($f > 2f_c$) [11], and the front of totally failed elements [21]. Here, a modification of the proposal of Seupel and Kuna [21] is applied, which can be easily performed in case of 2D plane strain analysis. The crack extension is defined considering two typical states: i) crack tip blunting and growth of voids until crack formation, and ii) crack growth due to total material failure:

$$\Delta a = \begin{cases} 
\Delta a_{blunt} + \Delta a_{dam} & \max(f) < f_u \\
\Delta a_{blunt} + \Delta a_{fail} & f_u \leq \max(f)
\end{cases}$$  \hspace{1cm} (17)

The blunting contribution $a_{blunt}$ is measured in the FE model as relative displacement along the ligament (vertical in the picture) between the FE nodes A and B highlighted in Fig. 1 b). Prior to total material failure, an averaged contribution $\Delta a_{dam}$ is added, which considers the formation and growth of voids.
Table 4: Parameter sets for sensitivity study

<table>
<thead>
<tr>
<th>Set</th>
<th>$f_0$</th>
<th>$f_c/f_0$</th>
<th>$k$</th>
<th>$l_{nl}$ in mm</th>
</tr>
</thead>
<tbody>
<tr>
<td>Reference</td>
<td>0.01</td>
<td>3</td>
<td>5</td>
<td>0.122</td>
</tr>
<tr>
<td>Variation $f_c/f_0$</td>
<td>0.01</td>
<td>[4.5, 6]</td>
<td>5</td>
<td>0.122</td>
</tr>
<tr>
<td>Variation $k$</td>
<td>0.01</td>
<td>3</td>
<td>[2, 3]</td>
<td>0.122</td>
</tr>
<tr>
<td>Variation $l_{nl}$</td>
<td>0.01</td>
<td>3</td>
<td>5</td>
<td>[0.2, 0.3]</td>
</tr>
<tr>
<td>Variation $f_0$ and $f_c/f_0$</td>
<td>[0.005, 0.015]</td>
<td>[3, 4.5, 6]</td>
<td>5</td>
<td>0.122</td>
</tr>
</tbody>
</table>

Figure 4: Variation of internal length $l_{nl}$: influence on a) force vs. diameter reduction of notched tensile test R4 and b) R-Curve of SENB-test (blunting line and its 0.2 mm offset included). Experimental data from [24, 25, 23].

The location $x_{dam}$ of the first totally failed material point (integration point) in front of the initial crack tip (point B in Fig. 1 b) is extracted from the simulation. From B ($x = 0$) to $x_{dam}$, the crack extension is measured as averaged void volume fraction as introduced by Linse et al. [10], here with respect to the current configuration:

$$\Delta a_{dam} = \int_{0}^{x_{dam}} \frac{f^* - f_0}{f_u^* - f_0} d x.$$  \hspace{1cm} (18)

After the first total failure occurred, the distance $\Delta a_{fail}$ between point B and the front of total failure along the ligament is added to the crack tip blunting term in Eq. (17).

For comparison, the averaging method of Linse et al. [10]

$$\Delta a = \int_{0}^{W-a_0} \frac{f^* - f_0}{f_u^* - f_0} d x.$$  \hspace{1cm} (19)

and the evaluation of crack length using the partial unloading technique (B) are applied.

4.3.1. Sensitivity study

The sensitivity study is performed for the SENB-test, which should deliver the main information on choosing the model parameters according to the proposed calibration strategy. Additionally, the influence of varied model parameters on the response of notched tensile tests is discussed, here for R4. Please note that the obtained results on notched tensile test from sensitivity study are not used for model calibration in the following.
The varied parameters and the variation range are summarized in Tab. 4. The reference set is motivated by the work of Hütter et al. [20] \( (f_0, f_c \text{ and } k) \). The suggestion \( l_{ad} = 0.122 \text{ mm} \) is taken from the model of Seupel and Kuna [21] considering the same material.

In Figs. 4–6, the influence of varied model parameters on the force \( F \) vs. diameter reduction \( -\Delta d/d_0 \) response of the notched tensile test and R-curves of the SENB-test are illustrated. Experimental results are added for a first comparison. The R-curves exhibit a characteristic course: Firstly, they coincide with the blunting line, due to definition (17), followed by a range of strongly changed curvature between the blunting line and its 0.2 mm offset. In this stage, no total material failure occurs. The first total failure of a material point is characterized by the horizontal tangent near to the 0.2 mm offset line. This jump-in like behavior is due to the fact that first total failure occurs in some distance to the initial crack tip [10]. Basically, the shapes of the R-curves are comparable to the simulation results of Hütter et al. [20].

The fracture initiation toughness (deviation from blunting line or intersection with 0.2 mm offset) can be adjusted by changing the internal length \( l_{ad} \), see Fig 4 b). The tearing modulus (slope of the R-curve) is not affected, which is in accordance with findings in [20]. In case of the notched tensile test, the increase of internal length delays the pronounced softening branch of the \( F \) vs. \(-\Delta d/d_0 \) curve. The slope of the softening branch is not changed.

The variation of the parameter \( k \), which controls the accelerated void growth, exhibits a similar effect on the R-curve as the internal length. Increasing \( k \) yields a lower initiation toughness, see Fig 5 b). In contrast to the internal length, a change of \( k \) shifts the onset of pronounced softening and leads to slightly different slopes in the result of the notched tensile test (Fig. 5 a)).

Simulated R-curves for different sets of initial and critical porosities, \( f_0 \) and \( f_c \), respectively, are shown in Fig. 6 b)–d). The same ratios \( f_c/f_0 \) are considered for fixed \( f_0 \). Increasing the ratio \( f_c/f_0 \) increases the tearing modulus in all cases. Simultaneously, the fracture initiation toughness is elevated. Moreover, same ratios \( f_c/f_0 \) for different initial porosities \( f_0 \) yield nearly the same trend. According to Hütter et al. [20], the tearing modulus should be highly influenced by the critical porosity \( f_c \). However, the discussed R-curves in Fig. 6 b)–d) imply a more precise conclusion: the ratio \( f_c/f_0 \) is mainly relevant for tearing modulus if different values of \( f_0 \) are used. Due to the vanishing impact of \( l_{ad} \) and \( k \) on the tearing modulus, a unique calibration is possible by adjusting \( f_c/f_0 \). For the notched tensile test, the variation of \( f_c/f_0 \) leads to a shift of the steep softening branch with minor change in slope, see Fig. 6 a).

At this point, the calibration strategy proposed in Sec. 3.3 can be validated and refined: a unique calibration of the internal length \( l_{ad} \) and the ratio \( f_c/f_0 \) will be possible if \( k \) and \( f_0 \) are fixed. It is

\[ \text{Figure 5: Variation of acceleration parameter } k: \text{ influence on a) force vs. diameter reduction of notched tensile test R4 and b) R-Curve of SENB-test (blunting line and its 0.2 mm offset included). Experimental data from [24, 25, 23].} \]
Figure 6: Variation of ratio \( f_c/f_0 \): influence on a) force vs. diameter reduction of notched tensile test R4 and b)–d) R-Curves of SENB-test with different initial porosities \( f_0 \) (blunting line and its 0.2 mm offset included). Experimental data from [24, 25, 23].

expected that appropriate parameter sets can be found if slightly different values for \( f_0 \) and \( k \) are assumed. If results of notched tensile tests are available, \( k \) can be estimated by fitting the slope of the rapid softening branch of force vs. diameter reduction curves. Nonetheless, a substantial improvement is not expected, i.e., the choice of \( k \) does not seem to play a major role.

However, some practical reasons should be taken into account for the choice of \( k \): Low values of \( k \) possibly necessitate a small internal length \( l_{id} \), which can be concluded especially from the case \( k = 2 \) in Fig. 5 b). A small internal length requires a fine discretization due to the convergence condition \( l_{id} \leq 1/4 l_{id} \), which increases the computational costs. On the other hand, a high value of \( k \) can result in a higher number of incremental steps during numerical solution: Let’s assume a constant stress triaxiality during loading at integration point level. Faster softening, i.e., lower stresses, are reached at same deformation states for high values of \( k \) compared to low ones after exceeding \( f_c \). Therewith, smaller increments for displacement controlled FEM-simulations become necessary due to possible numerical convergence issue within the material subroutine. During preparation of the present study, \( 2 \leq k \leq 5 \) is found to be a compromise.

4.3.2. Calibration results

A close inspection of the simulated R-curve results and the experimental data during sensitivity analysis infers that an appropriate solution may be found near to the investigated parameter sets. In order to study the influence of slightly varied starting values on model predictions, three sets with fixed pairs of
Table 5: Sets of calibrated parameters. The bold entries are fixed during optimization.

<table>
<thead>
<tr>
<th>Set</th>
<th>$f_0$</th>
<th>$f_c/f_0$</th>
<th>$k$</th>
<th>$l_{nl}$ in mm</th>
</tr>
</thead>
<tbody>
<tr>
<td>#1</td>
<td>0.01</td>
<td>6</td>
<td>5</td>
<td>0.12</td>
</tr>
<tr>
<td>#2</td>
<td>0.01</td>
<td>7</td>
<td>4</td>
<td>0.1</td>
</tr>
<tr>
<td>#3</td>
<td>0.005</td>
<td>9.0</td>
<td>4</td>
<td>0.075</td>
</tr>
</tbody>
</table>

Figure 7: Comparison of R-curves: a) experiment vs. simulations with calibrated parameter sets from Tab. 5 and b) R-curves for different mesh refinements $b_c/l_{nl}$ with parameter set #2. Experimental data from [23].

Figure 8: Convergence study SENB-test: Distribution of void volume fraction $f^*$ for different mesh refinements $b_c/l_{nl}$ at a crack extension of $\Delta a=1.2\, \text{mm}$. Simulations are conducted with parameter set #2 from Tab. 5; $f_0 = 0.01$, $f_c = 0.07$. Integration points with $f^*$ between $f_u^* = 0.98/q_1$ and $f_{\text{max}}^* = 0.995/q_1$ are considered as totally damaged (highlighted in purple).
Figure 9: Predictions of the a) force vs. diameter reduction and b) force vs. elongation response of the notched and smooth tensile tests using pure $J_2$-plasticity ($f_0 = 0$) with hardening law (16) and parameters given in Tab. 3. Dashed lines correspond to experiments, solid lines correspond to simulations. Experimental data from [24, 25].

$f_0$ and $k$ are assumed as summarized in Tab. 5. Set #1 and #2 use a relatively high initial porosity of 1%, but different $k$-values. Set #3 starts with an initial porosity of 0.5%. The determined parameters ($f_c, l_0$) are given in Tab. 5 and the comparison to the experimental $R$-curve is shown in Fig. 7 a). The calibrated curves of the different sets nearly coincide. A good fit of the technical fracture initiation toughness at 0.2 mm blunting line offset and beyond is found. As expected, using a low value of $k$ leads to a low internal length, see Tab. 5. Set #3 with smallest $f_0$ exhibits an even smaller internal length. Thus, the internal length of the proposed non-local GTN-model is not a fixed material parameter, but rather an adjustable model parameter. However, its calibrated size $\approx 100 \mu$m lies in the order of magnitude of the steel’s grain size ($\approx 125 \mu$m).

In order to underline the regularization properties of the non-local GTN-approach, a convergence study is performed for the crack growth simulations of the SENB-test with the calibrated model (set #2). In Fig. 7 b), the resulting $R$-curves are plotted for different mesh refinements $h_c/l_0$. The coarsest mesh $h_c/l_0 = 1/2$ gives a slight overestimation in comparison to the curves $h_c/l_0 \leq 1/4$ which perfectly coincide. Furthermore, Fig. 8 illustrates the distribution of the effective void volume fraction $f^*$ for the different meshes at a crack extension of $\Delta a = 1.2$ mm. The distribution of $f^*$ is similar for all mesh refinements. It should be mentioned that no spurious widening of the total damaged zone ($f^* \geq f^*_{\text{u}}$) can be observed due to the damping effect of the proposed patch solution of handling total material failure, see Sec. 2.2. Hence, the meshing recommendation $h_c/l_0 \leq 1/4$ from literature as well as the regularization ability of the proposed damage model are confirmed.

4.4. Validation

In Fig. 9, simulation results of the notched tensile tests are shown, which are obtained applying pure $J_2$-plasticity ($f_0 = 0$). For all notched tensile tests, a good agreement of force response with respect to elongation and diameter reduction is found up to the sudden onset of pronounced softening indicated by kinks in the experimental curves. Therewith, the proper choice of the strain hardening law is underpinned, which allows for reasonable predictions during the stage of diffuse necking.

The final task of the calibrated non-local GTN-model is to predict the deviation point in the force response, i.e., the rather sudden load drop. All three determined sets of parameters (Tab. 5) are used to simulate the failure behavior of smooth and notched tensile tests, Fig. 10, as well as the small punch test, Fig. 12.

Firstly, the predictions of tensile tests are discussed. At a glance, all calibrated sets give reasonable
predictions of the prominent failure point, i.e., the onset of pronounced softening, see Fig. 10. This is true for the force vs. diameter reduction and elongation curves, respectively. It should be emphasized that also failure of the smooth tensile test is nearly matched. Using set #3 with the initial porosity \( f_0 = 0.005 \) yields a slight overestimation of the experimentally observed failure initiation in the force vs. diameter reduction response of the notched tensile tests. But the prediction is still acceptable from an engineering point of view. Choosing \( k = 4 \) (set #2 and #3) yields a better agreement of the steep softening parts in force vs. diameter reduction curves of the notched tensile tests.

Although a high initial porosity of 1% is assumed in sets #1 and #2, which is surely not realistic for modern steels, just slight deviations of simulated from experimental force displacement curves can be found. Thus, for future application of the proposed non-local GTN-model to high strength steels with similar hardening and deformation characteristics, an initial porosity \( f_0 = 0.01 \) can be taken into account as first guess.

The simulated deformation state of the initially smooth tensile test at crack formation and total failure is compared to the experimental result in Fig. 11 a)–c). A diffuse necking occurs prior to crack formation, which is captured by the simulation. The crack propagates from the specimen’s center to the boundary in a straight manner. On the surface of the real specimen, a slight zig-zag form of the crack in circumferential direction can be detected, which cannot be reproduced with the utilized rotationally symmetric FE-model. However, no pronounced cup-cone fracture mode can be reported (not visible in the picture), which makes the model prediction acceptable.

In Fig. 12, the predictions of the force vs. displacement curves from SPT-simulations are compared to experimental data. No significant difference is observed between the calibrated parameter sets. A slight overestimation of the upper bound curve from experiments is visible for all predictions up to a punch displacement of \( \approx 1 \) mm. The GTN-simulations do not show a significant deviation in comparison to the simulation with pure \( J_2 \)-plasticity. Again, the proper choice of the strain hardening law is underpinned, as already mentioned by Seupel and Kuna [21]. The onset of pronounced load drop is overestimated by the GTN-model, although the maximum force is in good agreement. Softening is also observed for the \( J_2 \)-plasticity simulation due to necking, however, far beyond the experimental onset point. It should be emphasized that the SPT exhibits the lowest stress triaxiality \( h = \sigma_{h}/\sigma_{eq} \) at the location of crack formation of all considered tests, with \( h \approx 2/3 \) see Seupel and Kuna [21]. The smooth tensile test starts with \( h = 1/3 \). But after onset of diffuse necking, values around \( h = 4/5 \) are reached. Void growth is assumed within this study as dominant damage mechanism, which is true at high stress triaxialities. However, concerning the results of SPT, the predictive power and validity of a purely void growth based GTN-model becomes questionable for \( h \leq 2/3 \).

The fracture mode of simulated SPT is compared to the experimental result in Fig. 11 d)–e). The simulation is evaluated at the loading point of finished crack formation, cf. Fig. 12. The location of the final crack with respect to the vertical axis is in accordance with the experimental finding. However, Fig. 11 e) shows that the final crack does not uniformly occur around the circumference in experiments. This feature is not reflected by the simulation, because rotational symmetry is assumed for the FE-model. Further investigations using 3D-models are necessary in order to generate such a fracture pattern.

Finally, we consider the impact of different crack extension definitions on the predicted failure behavior. For the calibrated parameter set #2, the simulated R-curve is recalculated with \( \Delta a \) as output from the averaging method, Eq. (19). The results are plotted in Fig. 13. The different evaluation methods for \( \Delta a \) do not lead to evident deviations of the R-curves beyond the 0.2 mm offset of the blunting line. The averaging method yields a self-similar, but slightly right-shifted R-curve in comparison to the reference method (Eq. (17)). The averaging method deviates near the blunting line and the horizontal tangent in the R-curve at first material failure is not visible. Nonetheless, using values beyond 0.2 mm offset of blunting line for calibration would yield similar model parameters.

If the partial unloading technique is used following the experimental procedure, lower \( \Delta a \) values at same global loading point are obtained in comparison to both other methods. Therefore, the data points \( J - \Delta a \) are shifted to the left leading to an apparently higher crack resistance, see Fig. 13. In the specific
Figure 10: Failure predictions of the a)-c) force vs. diameter reduction and d)-f) force vs. elongation response of the notched and smooth tensile tests for the three parameter sets from Tab. 5. Dashed lines correspond to experiments, solid lines correspond to simulations. Experimental data from [24, 25, 23].
Figure 11: Simulated and experimental failure patterns of a)–c) smooth tensile test and d)–e) small punch test (SPT): a) crack formation state, b) final failure, d) snapshot at the end of crack formation (see Fig. 12). The pictures from simulation show a cut through the specimens. Note: The pictures are manipulated FE-results (mirrored, rotated) for visualization purposes.

Figure 12: Prediction of the force vs. punch displacement response of the small punch test (SPT) using the parameter sets #1–#3 from Tab. 5. Experimental lower (LB) and upper bound (UB) are shown. The cross \( \times \) designates the end of crack formation \([24]\). The simulation without damage is additionally considered. Experimental data from \([24, 25]\).
case, if the partial unloading method is used to calibrate the non-local GTN-model, a lower value of the internal length $l_{nl}$ would be necessary in order to fit the experimental R-curve. Interestingly, the tearing moduli of the different evaluation methods are nearly the same. The definition of $\Delta a$ by partial unloading yields a conservative choice, whereas both other methods do not differ substantially. Please note that the evaluation using partial unloading highly depends on the correct compliance function of the testing setup and material (see B).

5. Conclusions

A regularized GTN-model is investigated, where softening due to void growth is based on a non-local volumetric plastic strain. A simple implementation of the model into the commercial FE-code ABAQUS is proposed. The model is calibrated and validated with help of experiments conducted for a pressure vessel steel at moderate to high stress triaxialities. Monotonic loading scenarios with dominant Mode I crack growth are considered.

Firstly, some general conclusions can be drawn:

- The non-local GTN-model can be calibrated using results of a uni-axial tensile test and a fracture mechanics test considering Mode I crack growth, here SENB-test.
- If the considered material exhibits diffuse necking with a small ratio of uniform to total elongation, the choice of strain hardening law will have a significant influence on simulated response of smooth and notched tensile tests. Therefore, FE-simulations of the smooth tensile test should be used to assess the suitability of different strain hardening laws during model calibration.
- According to the strategy proposed by the authors in [20], a unique calibration of internal length $l_{nl}$ and critical porosity $f_{c}$ is possible. However, $k$ (coefficient of accelerated void growth) and the initial porosity $f_{0}$ have to be fixed in advance.
• The critical void volume fraction $f_c$ and the internal length $l_{nl}$ can be identified from crack growth resistance curves. They influence the tearing modulus and fracture initiation toughness, respectively. Same ratios $f_c/f_0$ for slightly different initial porosities $f_0$ yield comparable tearing moduli. In contrast to the conclusions of Hütter et al. [20] and the present results, the critical porosity $f_c$ is fixed beforehand in other studies dealing with calibration of non-local GTN-models, e.g., [11].

• A low influence of $k$ on the slope of simulated R-curves is revealed. Force vs. diameter reduction curves of notched tensile tests can help to reasonably choose $k$. The proposed range $2 \leq k \leq 5$ is furthermore motivated by computational reasons.

• Two methods to extract the crack extension from 2D-simulation data are tested: averaging of porosity along the ligament and picking the front of total material damage as crack tip. Both methods yield equivalent calibration results.

• Interestingly, a simulation of the experimentally applied technique of partial unloading is possible to determine the crack extension with the non-local GTN-model. The results do not severely differ in comparison to the other proposed methods for defining crack extension.

Furthermore, conclusions are drawn for the applicability of the non-local GTN-model concerning the specific pressure vessel steel 18Ch2MFA (comparable to 17CrMoV 9 [22]) and considered loading states as follows:

• The GTN-model yields excellent failure predictions of notched and smooth tensile tests.

• For different initial porosities $0.005 \leq f_0 \leq 0.01$ one can find appropriate sets of model parameters related to material softening ($f_c$, $l_{nl}$, $k$) yielding equivalent predictions.

• Although the assumption of $f_0 = 0.01$ is not realistic for modern steels, an acceptable behavior is obtained for the considered pressure vessel steel.

• Due to the good model predictions, the necessity of an additional void nucleation term is not given. Thus, parameters can be omitted which are typically difficult to identify, e.g., the strain controlled nucleation law of Chu and Needleman [2].

• On the other hand, if stress triaxialities $h \leq 2/3$ occur at the crack formation site, the predictions will be less accurate. This indicates that the applicability of the purely void growth based GTN-model is restricted to high stress triaxiality.

In order to further underpin and validate the findings concerning the utilized non-local GTN-model, the same calibration strategy should be applied to other materials in future works. Simulations and experiments on fracture mechanics specimens with different constraint would be helpful for further assessment of the model, as it was done by Zhang et al. [11].

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A. Implementation aspects

In the FE-implementation, the similarity of the steady state heat equation

\begin{equation}
\lambda_h \Delta x \vartheta + p_{th} = 0 \quad \forall \vartheta \in \Omega, \tag{20}
\end{equation}

and the gradient-enhanced setting (Eq. (7)-(8)) is utilized as proposed by Seupel et al. [15]. The temperature degree of freedom is interpreted as non-local variable \( \bar{\varepsilon}_h \leftrightarrow \vartheta \). The strain and temperature dependent heat source \( p_{th} \) is identified as the difference \( -\bar{\varepsilon}_h + \varepsilon_{th} \leftrightarrow p_{th} \). Finally, the conductivity \( \lambda_{th} \) is renamed as the internal length squared \( l_{th}^2 \leftrightarrow \lambda_{th} \). Therewith, the subroutines UMAT/HETVAL of ABAQUS can be used to define the stress \( \sigma \) and pseudo heat source \( p_{th} \) as well as the consistent material tangent.

The integration of the hypoelastic relation (1) is explained elsewhere, e.g., see [15]. In the following, matrix-vector notation is introduced, where a symmetric second-order tensor \( \mathbf{A} \) is handled as algebraic column vector \( \mathbf{A} \) and a fourth-order tensor \( \mathbf{A} \) with certain symmetries is expressed as algebraic matrix \( \mathbf{A} \). The matrix multiplication is denoted by a center dot (\( \cdot \)); the transpose is highlighted by superscript \( T \), the inverse by superscript \( -1 \). The reader is referred to [15] for more details. In what follows, a superscript \( n \) refers to a known value from the previous incremental step. The index for the new state \( n+1 \) is omitted.

The primary input variables of the material routine UMAT are the strain increment \( \Delta \varepsilon \) and the increment of the non-local variable \( \Delta \bar{\varepsilon}_h \) as well as \( \bar{\varepsilon}_{th} \). As output, the new stress \( \sigma \) and the new pseudo-heat source \( p_{th} \) have to be calculated, both as functions of \( \Delta \varepsilon \) and \( \Delta \bar{\varepsilon}_h \). As mentioned above, the corresponding consistent material tangents \( \{ K_{se}, K_{st}, K_{pe}, K_{pt} \} \) have to be provided as additional output of the subroutines UMAT/HETVAL as explained in detail in [15, 39]. The specific definitions of the tangent entries are given below in Eq. (26).

The stress is to be updated according to

\begin{equation}
\sigma = \sigma^{tr} - C \cdot \Delta \varepsilon_{pl}, \tag{22}
\end{equation}

where the trial stress \( \sigma^{tr} \) is defined as

\begin{equation}
\sigma^{tr} = \sigma^{rot} + C \cdot \Delta \varepsilon. \tag{23}
\end{equation}

The superscript \( "tr" \) highlights values directly calculated from the trial stress \( \sigma^{tr} \). The rotated stress from last increment \( \sigma^{rot} \) is provided as UMAT’s input. The plastic rate of deformation (4) is integrated by the Euler-backward method, which yields the plastic strain increment

\begin{equation}
\Delta \varepsilon_{pl} = \Delta \varepsilon_{eq}^{tr} + \Delta \varepsilon_{th} \delta. \tag{24}
\end{equation}

Moreover, the Euler-backward scheme is applied to all considered evolution equations.

In addition to the new stress, the pseudo heat source has to be updated:

\begin{equation}
p_{th} = -(\bar{\varepsilon}_{th} + \Delta \bar{\varepsilon}_h) + \bar{\varepsilon}_{th} + \Delta \bar{\varepsilon}_h. \tag{25}
\end{equation}

Therein, \( \Delta \bar{\varepsilon}_h \) is the increment in local volumetric plastic strain.
For the global solution during FE-simulation, a Newton-scheme is utilized, which requires the calculation of the consistent material tangent. In case of the coupled mechanical-non-local problem the specific entries read

\[ K_{\text{co}} = \frac{\partial \sigma}{\partial \Delta \bar{E}} + \frac{1}{J} \sigma \cdot \left( \frac{\partial J}{\partial \Delta \bar{E}} \right), \quad K_{\text{st}} = \frac{\partial \sigma}{\partial \Delta \varepsilon}, \quad K_{\text{pe}} = \left( \frac{\partial p_{\text{h}}}{\partial \Delta \varepsilon_h} \right)^T, \quad K_{\text{pt}} = \frac{\partial p_{\text{h}}}{\partial \Delta \varepsilon_h}. \]  

\[ (26) \]

\( K_{\text{co}} \) is the non-symmetric stress tangent as demanded by ABAQUS. \( K_{\text{st}}, \) \( K_{\text{pe}}, \) and \( K_{\text{pt}} \) are the derivatives of stress with respect to change in non-local variable and the derivatives of the pseudo heat source with respect to \( \Delta \bar{E} \) and \( \Delta \varepsilon_h. \)

The determinant of the deformation gradient \( J \), which is related to volume change, and its derivative are given by [15]

\[ J = J^n \exp \left( \delta^T \cdot \Delta \bar{E} \right), \quad \frac{\partial J}{\partial \Delta \bar{E}} = J \delta^T. \]

The rate independent model is handled with an established operator split, also applied in [15, 21]. Hence, the yield function \( \Phi \) is evaluated with fixed internal variables \( (r^n) \), the trial state characterized by \( \sigma^n \), and the new porosity, whose discretized evolution equation yields

\[ f = 1 - (1 - f_0) \exp (-3 (r^n + \Delta r)), \quad f^* = f^* (f). \]

The increase in \( \Delta \varepsilon_h \) is given by solving the discrete formulation of Eq. (11). Note that the porosity is always updated, even in the elastic case since \( \varepsilon_h \) may evolve from plastic deformation in the neighborhood.

A.1. Elastic response

For \( \Phi (\sigma^n, r^n, f^*) < 0 \), the stress and pseudo heat source are updated using the trial state and \( \Delta \varepsilon_h = 0. \) The consistent material tangent yields

\[ K_{\text{co}} = C + \frac{1}{J} \sigma \cdot \left( \frac{\partial J}{\partial \Delta \bar{E}} \right), \quad K_{\text{st}} = 0, \quad K_{\text{pe}} = 0^T, \quad K_{\text{pt}} = -1 \]

\[ (29) \]

A.2. Elastic-plastic response

For the elastic plastic response \( (\Phi (\sigma^n, r^n, f^*) \geq 0) \), the radial return method proposed by Aravas [40] is utilized. The system of equations can be reduced to two unknowns: \( \Delta \varepsilon_{\text{eq}} \) and \( \Delta \varepsilon_h. \) The equations to be solved stem from the yielding condition \( \Phi = f_1 = 0 \) and from eliminating the plastic multiplier \( \Lambda_{\text{pt}} \) by combining the two equations given in Eq. (5) [40]:

\[ f_1 = \frac{(\sigma_{\text{eq}}^n - 3G\Delta \varepsilon_{\text{eq}})^2}{\sigma_y^2} + 2q_1 f^* \cosh \left( \frac{3q_2 (\sigma_{\text{eq}}^n - 3K \Delta \varepsilon_h)}{2\sigma_y} \right) - \left( 1 + (q_1 f^*)^2 \right) = 0 \tag{30} \]

\[ f_2 = \frac{2 (\sigma_{\text{eq}}^n - 3G\Delta \varepsilon_{\text{eq}})}{\sigma_y^2} \Delta \varepsilon_h - q_1 q_2 f^* \sinh \left( \frac{3q_2 (\sigma_{\text{eq}}^n - 3K \Delta \varepsilon_h)}{2\sigma_y} \right) \Delta \varepsilon_{\text{eq}} = 0. \tag{31} \]

The non-linear system of equations is solved by a standard Newton-Raphson-method.

The numerical integration of the rate of hardening (6) cannot be solved for \( \Delta r \) directly. A nested scheme is applied: During every iteration of the Newton-Raphson scheme to solve \( f_1 \) and \( f_2, \) the additional non-linear equation in \( \Delta r \)

\[ f_3 = -\Delta r + \frac{(\sigma_{\text{eq}}^n - 3G\Delta \varepsilon_{\text{eq}}) \Delta \varepsilon_{\text{eq}} + 3 (\sigma_{\text{eq}}^n - 3K \Delta \varepsilon_h) \Delta \varepsilon_h}{(1 - f^n - \Delta f) \sigma_y (r^n + \Delta r)} = 0, \tag{32} \]

\[ (32) \]
given by numerical integration of (6), is solved by a Newton-Raphson scheme for fixed \( \Delta \varepsilon_{eq}, \Delta \varepsilon_h \).

The tangent stiffness \( T \) and the right-hand-side vector \( R \) for numerical solution of (30)-(31) via Newton-Raphson scheme read

\[
T = \begin{bmatrix}
\frac{\partial f_1}{\partial \Delta \varepsilon_{eq}} & \frac{\partial f_1}{\partial \Delta \varepsilon_h} \\
\frac{\partial f_2}{\partial \Delta \varepsilon_{eq}} & \frac{\partial f_2}{\partial \Delta \varepsilon_h}
\end{bmatrix}, \quad R = -\begin{bmatrix} f_1 \\ f_2 \end{bmatrix}.
\]

The required derivatives \( \partial \Delta r / \partial \Delta \varepsilon_{eq} \) and \( \partial \Delta r / \partial \Delta \varepsilon_h \) somewhere hidden in \( T \) are obtained by implicit differentiation of \( f, \) Eq. (32).

The final stress update reads

\[
\sigma = \sigma^{tr} - C \cdot (\Delta \varepsilon_{eq} \mathbf{N}^{tr} + \Delta \varepsilon_h \delta).
\]

A.3. Consistent material tangent

The total differentials of Eq. (34) and (25) with respect to the input variables \( \sigma^{tr} \) and \( \Delta \varepsilon_h \) intermediately read

\[
d \sigma = d \sigma^{tr} - C \cdot (d \Delta \varepsilon_{eq} \mathbf{N}^{tr} + d \Delta \varepsilon_h \delta),
\]

\[
d \rho_{th} = -d \Delta \varepsilon_h + d \Delta \varepsilon.
\]

The total differential of the trial yield normal reads

\[
d \mathbf{N}^{tr} = \mathbf{P} \cdot d \sigma^{tr} = \frac{3}{2 \sigma_{eq}^{tr}} \left( \mathbf{T} - \frac{1}{3} \delta \cdot \delta^T - \frac{3}{2 (\sigma_{eq}^{tr})^2} \mathbf{S}^{tr} \cdot \left( \mathbf{S}^{tr} \right)^T \cdot \mathbf{P} \right) \cdot d \sigma^{tr},
\]

with the unity matrix \( I \) and the scaling matrix \( P \), see [15].

The total differentials \( \langle d \Delta \varepsilon_{eq}, d \Delta \varepsilon_h \rangle \) are obtained for the converged state of the Newton-Raphson scheme from \( d f_1 = 0 \) and \( d f_2 = 0 \) (Eq. (30) and (31)) as

\[
T \cdot \begin{bmatrix} d \Delta \varepsilon_{eq} \\ d \Delta \varepsilon_h \end{bmatrix} = U d \Delta \varepsilon_h + V \cdot d \sigma^{tr}.
\]

The right-hand-side is constituted with help of

\[
U^T = -\begin{bmatrix}
\frac{\partial f_1}{\sigma^{tr}} & \frac{\partial f_2}{\sigma^{tr}}
\end{bmatrix} \cdot \frac{\partial f}{\partial \Delta \varepsilon_h},
\]

\[
V = -\begin{bmatrix}
\left( \frac{\partial f_1}{\sigma^{tr}} \right)^T \\
\left( \frac{\partial f_2}{\sigma^{tr}} \right)^T
\end{bmatrix}.
\]

The solution of (38) is given by Cramer’s rule:

\[
\begin{bmatrix} d \Delta \varepsilon_{eq} \\ d \Delta \varepsilon_h \end{bmatrix} = \frac{1}{\det (T)} \text{adj} (T) \cdot (U d \Delta \varepsilon_h + V \cdot d \sigma^{tr}) = \begin{bmatrix} D_{eq} \\ D_h \end{bmatrix} d \Delta \varepsilon_h + \begin{bmatrix} D_{eq}^T \\ D_h^T \end{bmatrix} \cdot d \sigma^{tr}.
\]

According to Eq. (26), the variation with respect to the strain increment \( \Delta \varepsilon \) is required for the material tangent. Hence, the relation

\[
d \sigma^{tr} = C \cdot d \varepsilon
\]

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Figure 14: a) Force $F$ vs. crack mouth opening displacement $v$ and b) normalized compliance $C$ vs. $v$ during SENB-simulation with partial unloading. The arrows highlight the loading step which exhibits the lowest compliance $C_0$ used for calculation of crack extension $\Delta a$.

B. Simulation of partial unloading technique

The partial unloading technique is based on the fact that specimen compliance is changed during crack extension. The procedure follows mainly the ESIS-standard [34] and modifications proposed in [41]. During simulation, unloadings of $\approx 5\%$ with respect to the current force during loading are prescribed, see Fig. 14 a). The specimen compliance $N$ is determined from starting and end points of the unloading step. Afterwards, the normalized compliance $C$ is calculated via

$$ C = NB_e E' , \quad E' = \frac{E}{1 - \nu^2} , \quad B_e = B - \frac{(B - B_0)^2}{B} . $$

The compliance function to determine the crack length ratio $a/W = f(C)$ cannot be taken from standards, because a modified four-point-bending setting is utilized. In [42, 41], the compliance function for the four-point-loading of SENB-specimen is determined as

$$ \frac{a}{W} (C) = 0.118 + 2.256 \cdot 10^{-2} C - 5.14 \cdot 10^{-4} C^2 + 7.307 \cdot 10^{-6} C^3 $$
$$ - 5.691 \cdot 10^{-8} C^4 + 1.852 \cdot 10^{-10} C^5 . $$
for high strength steels comparable to 18Ch2MFA. The force $F$ vs. crack mouth opening displacement $v$ response is used to determine the compliance $N$, where $v$ is measured at the specimen surface (point $M$ in Fig. 1).

In Fig. 14 b), the course of normalized compliance with increasing crack mouth opening is plotted. Obviously, the compliance decreases during first loading steps and stabilizes around $v \approx 0.4...0.6$ mm. This behavior is known from experiments [41] indicating an apparently negative crack extension, although no total material damage can be found in simulated results. Fischer and Pusch [41] suggest to take the minimal compliance as reference to determine the initial crack length $a_0$, which is highlighted in Fig. 14 b). This point closely corresponds to the moment, where the critical porosity $f_c$ is exceeded near the crack tip as indicated by the simulation result. After this stage, the compliance $C$ monotonically increases, which is the result of stable crack propagation, i.e., the zone of total damage ($f^* \geq f^*_u$) extends along the ligament. The crack extension $\Delta a$ is finally calculated as

$$\Delta a = \left( \frac{a}{W} (C) - \frac{a}{W} (C_0) \right) W, \quad \text{for } C \geq C_0. \tag{50}$$

In order to complete the experimental procedure, a power law fit is applied to the data points within the exclusions lines, see Fig. 13, yielding

$$J = 408.5 \text{ N/mm} \left( \frac{\Delta a}{1 \text{ mm}} \right)^{0.27}. \tag{51}$$

References


