Improved Exploitation of High-strength Steels in Pressure Vessel Design by Simulations Based on Damage Mechanics

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Abstract Pressure vessels are subjected to regulation by European standards, which define design procedures and nominal material properties that are guaranteed by the steel producers. Over-conservative safety factors for materials with high yield-to-tensile ratios hinder the application of modern high-strength steels despite their excellent toughness and possible economic and ecologic benefits. Damage mechanics enable a more adequate failure description for these steels since they can consider ductile crack initiation as limit state. Such concepts should refer to nominal material characteristics to enhance their applicability in design procedures. A method is presented to correlate the nominal Charpy impact toughness to simulations with the Gurson-Tvergaard-Needleman-model (GTN). The resulting GTN parameters are used in cell model simulations to derive strain-based empirical failure criteria as nominal ductility measure for simulations on component level. A sensitivity study on the GTN parameter choice shows that the initial pore volume is the most relevant parameter, but other non-unique parameters also influence the failure prediction. The impact of the individual parameters is discussed. By the definition of a reliable calibration scheme for the GTN parameters this approach enables an identification of adequate lower bound failure criteria for high-strength steels in pressure vessels as a preliminary pressure vessel simulation demonstrates.

Keywords Strain-based Design, Pressure vessel, Damage mechanics, Damage curve

1. Introduction

In Europe, pressure vessels are subjected to regulation by the European Standard EN 13445, which contains the corresponding design rules. Additionally, the material requirements for pressure vessel steels are part of EN 10028. Therein, nominal material properties are defined, which specify minimum values for the mechanical properties. These have to be guaranteed by the steel producers and are often exceeded, especially by high quality steels. The nominal characteristics form the basis of the design process for pressure vessels. The required wall thickness is determined in dependence of the materials' nominal yield or tensile strength. The relevant design stress is specified in EN 13445 as the minimum of the yield strength divided by a safety factor of 1.5 or the tensile strength divided by 2.4. Therefore, the yield-to-tensile (Y/T) ratio determines the magnitude of the applied safety factor. From a Y/T-ratio of 0.625 on, the tensile strength with an increased safety factor of 2.4 is relevant for the design. Modern high strength steels are often characterised by such an increased Y/T-ratio, e.g. steel grade P500Q with Y/T = 0.85 and P690Q with Y/T = 0.9. By the application of the increased safety factor, only a poor exploitation of their load bearing capacity can be achieved. In this safety factor domain, the design stress is only 41% of the yield strength. Consequently, these rather expensive steel grades are rarely applied in pressure vessel design. However, their application would foster substantial economic and ecological benefits by e.g. thinner walls, which result in lower welding, energy and transportation cost.

The current safety factors are mainly based on experience and do not consider the actual failure behaviour [1]. Since EN 13445 requires brittle fracture to be excluded by the toughness requirements, an improved prediction of ductile crack initiation is needed. Hence, to improve the exploitation of high strength steels in pressure vessel design it is necessary to include a description of their ductility. The methods of damage mechanics are able to provide such predictions [2]. Although research on this field has been conducted for several decades, the methods of damage mechanics are not used regularly in industrial applications, let alone considered standard design procedures. One reason is that the application of damage mechanics models requires considerable expertise and experience since most of these models are strongly dependent on the non-unique parameter selection and the mesh size [2, 3]. A requirement for a safe and reliable use of damage mechanics models in pressure vessel design are therefore standardised application guidelines. Moreover, newly developed design criteria should be transferable to the standards and therefore need to refer to the nominal material properties. Currently, only yield and tensile strength are considered. The nominal property related to ductility is the minimum Charpy impact toughness. For example, EN10028-6 requires a nominal Charpy impact toughness of 60 J at room temperature for P500Q. Münstermann and Schruff have developed a method to determine ductile failure criteria for high strength pressure vessel steels out of these nominal characteristics [4, 5], which is further explained and discussed in the following.

2. A method for strain-based pressure vessel design with respect to nominal material properties

The ductile failure mechanism of metallic materials consists of the nucleation and coalescence of voids, which form under plastic deformation at inclusions [2]. This process is described by the damage model of Gurson, Tvergaard and Needleman (GTN). It was established by Gurson in 1977 [6] and is based on a continuum mechanics description of a hollow sphere in surrounding homogeneous material. Tvergaard and Needleman optimised the shape of the yield surface by the introduction of empirical fitting parameters [7]. The GTN model consists of a modified von Mises flow potential (Eq.1), and functions for the description of void nucleation (Eq.2) and coalescence (Eq.3).

(1)

(2)

(3)

The flow potential is a function of the equivalent stress σ_e, the hydrostatic stress σ_I, the empirical fit parameters q_i and the effective void volume fraction f^*. The latter is defined out of the nucleation function until the critical void volume fraction f_c is reached. Then the void growth is accelerated by the factor κ to account for the effects of void interaction. The nucleation function considers the plastic equivalent strain ε^{pl}, the volume fraction of possible nucleation sites for secondary voids f_N, the characteristic strain for nucleation of secondary voids ε_N as well as the standard deviation S_N.
The micromechanical motivation is one of the main advantages of this model. Some of its parameters, such as the initial void volume fraction, can be determined in metallographic analyses [2, 8]. This simplifies the parameter selection. Therefore, the GTN model is suitable to predict the crack initiation of high strength pressure vessel steels and is employed in the discussed approach.

However, the computational implementation of GTN requires too many resources for large scale component simulation as pressure vessel modelling. Therefore, a simpler model has to be applied in the component simulation. Such a model is the damage curve established by Johnson and Cook [9]. Depending on the evaluation procedure it describes the characteristic strain at failure or crack initiation as a function of stress triaxiality η, which is the ratio of hydrostatic to equivalent stress, and three constants c_i (Eq.4).

(4)

The damage curve can either be calibrated by experiments or by unit cell simulations based on the GTN model [10]. The unit cell (Fig. 1a) consists of one axisymmetric element, which is subjected to loads in two directions. By changing the ratio of the applied loads, it is possible to create different triaxiality states. Since the developed design approach shall be transferable to the standards it should refer to the nominal properties. An experimental calibration of the damage curve is only possible for a specific material of a single producer. Consequently, it allows no general application in standard design procedures. A derivation via unit cell simulations is a more general approach and is therefore applied.
The main idea of this approach is to re-calibrate an experimentally derived GTN parameter set for a specific steel grade in simulated Charpy tests [5]. The aim is to meet the nominal Charpy energy required in the standard for this steel grade. Such a set consequently characterizes the minimum ductile crack resistance. With this calibrated parameter set it is possible to determine a lower bound damage curve (Fig. 1b) for the simulation of ductile failure in pressure vessels with regard to nominal material properties [4, 5].

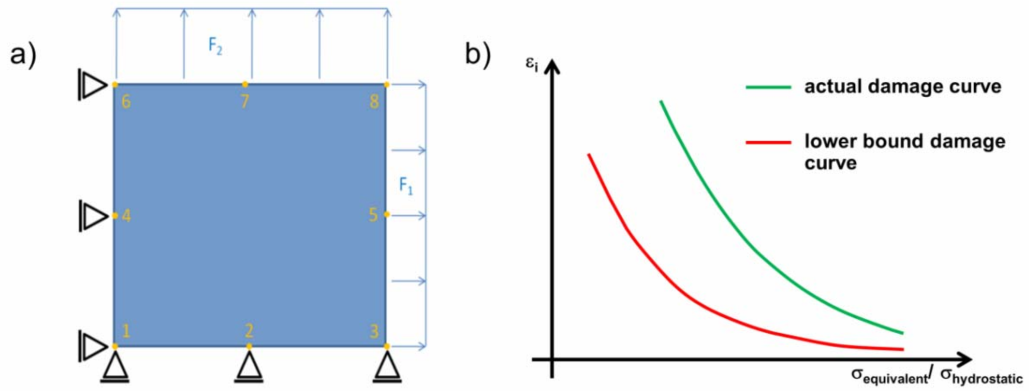


Figure 1. Schematic illustration of a) the axisymmetric unit cell and b) the damage curves.

The corresponding procedure based on [4, 5] consists of the following steps:

(1) Calibration of a suitable GTN parameter set and the corresponding mesh size for the selected material by metallography and an iterative optimisation process involving experimental and numerical results of notched round bar and fracture mechanics tests. Derivation of empirical functions for the materials strain rate and temperature dependence in an iterative process considering tensile tests at different temperatures and strain rates.
(2) Simulation of a Charpy impact toughness test with the determined values to validate the selection and the model and determine the corresponding friction value. Agreement between experimental and numerical results in overall energy and the course of the force-displacement curve shall be achieved.
(3) Derivation of the selected materials’ damage curve via unit cell simulations with varying stress triaxiality according to [5, 10].
(4) Calibration of a lower bound GTN parameter set in the simulation of a Charpy impact test with the aim to meet the nominal Charpy impact toughness specified in the standard for the selected material.

(5) Derivation of the lower bound damage curve via unit cell simulations with varying stress triaxiality according to [5, 10].
(6) Application of the lower bound damage curve in burst simulations for pressure vessels.

The burst simulation based on the lower bound damage curve allows a prediction of the failure onset in pressure vessels under consideration of the nominal Charpy impact toughness. These simulations can be part of an approach to derive more adequate safety factors for high strength pressure vessel steels. However, this approach can also be easily transferred to other applications fields subjected to regulation, e.g. civil engineering.

3. Influence of the non-unique GTN parameter selection on the course of the damage curve.

The developed concept contains the required steps for the identification of suitable GTN parameter sets. However, this selection is well-known to be non-unique [3, 8, 11]. It is therefore necessary to investigate the influence of the GTN parameter selection on the derived damage curve, since it represents the failure prediction element in the developed concept. Therefore, a sensitivity analysis is conducted with a GTN parameter set determined for the steel P500Q.
The reference set is derived by metallography and the comparison of numerical and experimental results of notched round bars in a tensile test. The relevant mesh size is determined in comparison to results of Compact-Tension-tests. The parameter set is validated in the simulation of a Charpy test. Details of the calibration procedure can be found in [5]. Unit cell calculations are performed with this reference set at stress triaxialities of 0.5, 1.0, 1.5, 2.0 and 2.5. The strain corresponding to the maximum stress in the unit cell is selected as critical strain for the derivation of the damage curve. At low stress triaxialities the GTN model may fail to predict softening, consequently no point for the damage curve can be derived.
During the sensitivity analysis one parameter is varied in the unit cell simulations while the others are kept constant. The calculations are performed at the above mentioned five stress triaxialities. Table 1 shows the reference parameter set determined for steel grade P500Q and the selected values for variation, which were chosen in accordance with literature [3, 11]. For q_3 the common relation $q_3 = q_1^2$ was applied in accordance with [7]. The aim of the sensitivity analysis is a qualitative description of individual parameters' influence on the damage curve. This description can form the basis for a rule set for the parameter derivation in the investigated approach.

Table 1. Reference set and variations for GTN parameters of steel P500Q

Parameter	f_0	f_N	S_N	ε_N	f_c	κ	q_1	q_2
Reference value	0.00185	0.00215	0.4	0.12	0.015	1.1	1.5	1.0
Maximum value	0.01	0.015	0.6	0.3	0.05	6	2.5	1.5
Minimum value	0.0005	0.0005	0.1	0.05	0.005	1	1	0.5
Mean value	-	-	-	-	-	3	-	0.8

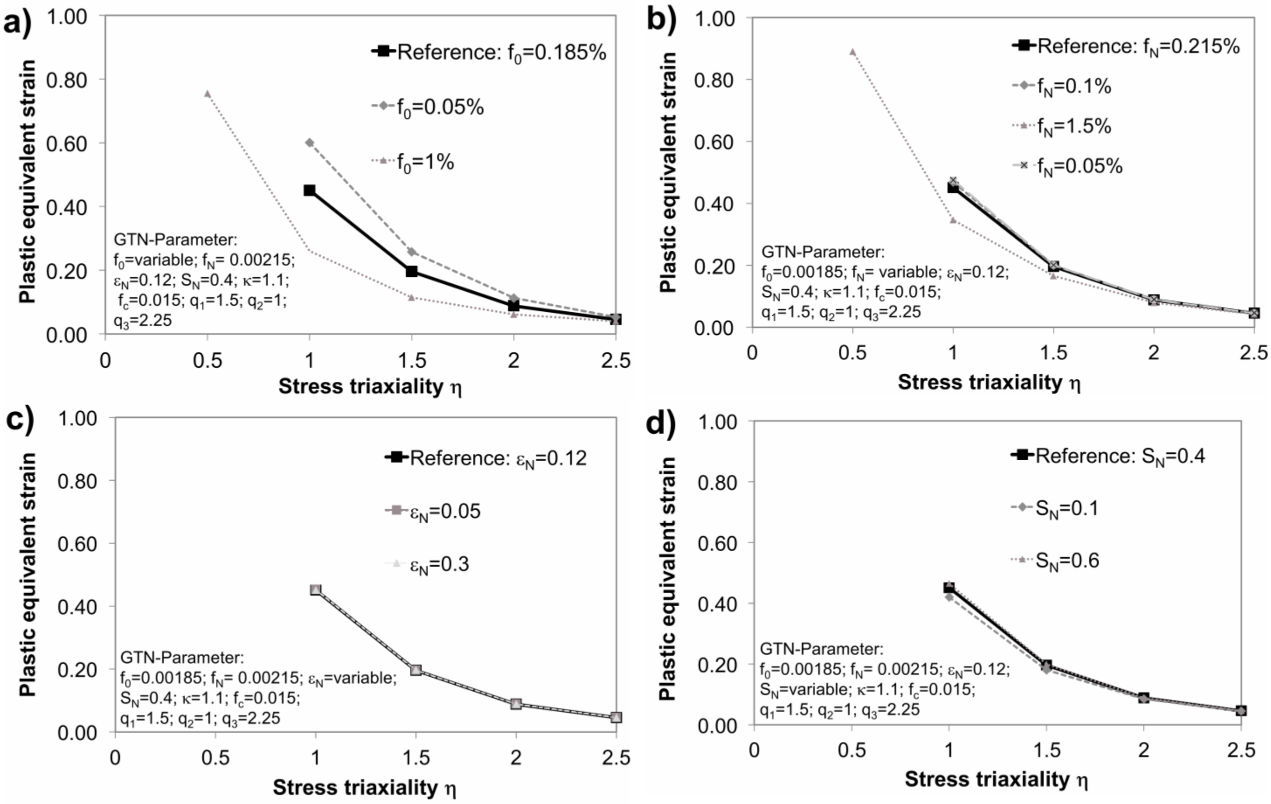
3.1. Results of the sensitivity analysis

3.1.1. Influence of f_0

The variation of the initial pore volume f_0 has a strong influence on the course of the damage curve, as can be seen in Fig. 2a. This effect increases with decreasing stress triaxiality. At a triaxiality of η=1, there is a maximum difference in critical strain of 34%. One reason for the strong impact of f_0 is that the initial pore volume influences the computation right from the beginning. This is also shown in Fig. 2e, which displays the equivalent stress in the unit cell and the effective void volume as a function of the equivalent strain for two triaxialities of η=1 and η=2.5. f_0 can very well be correlated to the volume content of non-metallic inclusions [5] and therefore be determined in metallographic analyses.

3.1.2. Influence of the void nucleation parameters f_N, ε_N and S_N

The void nucleation function (Eq.3) is based on a Gaussian distribution function. It is influenced by the volume fraction of possible nucleation sites for secondary voids f_N, the characteristic strain for nucleation of secondary voids ε_N and the corresponding standard deviation S_N. Consequently, these parameters interact. The secondary void volume f_N has a clear influence on the course of the damage curve at low triaxialities (Fig. 2b), the maximum difference at η=1 is 12%. However, this impact is lower than the one of f_0 although the input variation was comparable. Figure 2c and Figure 2d show that ε_N and S_N only have a minor influence on the predicted failure strains. This is due to the value of f_N, which limits the influence of ε_N and S_N. For many materials, the magnitude of f_N can also be determined in metallographic analyses. For the reference set it was determined as the volume fraction of carbides in P500Q. The minor influence of ε_N and S_N holds therefore true for realistic values of f_N, but it increases for higher values of f_N.



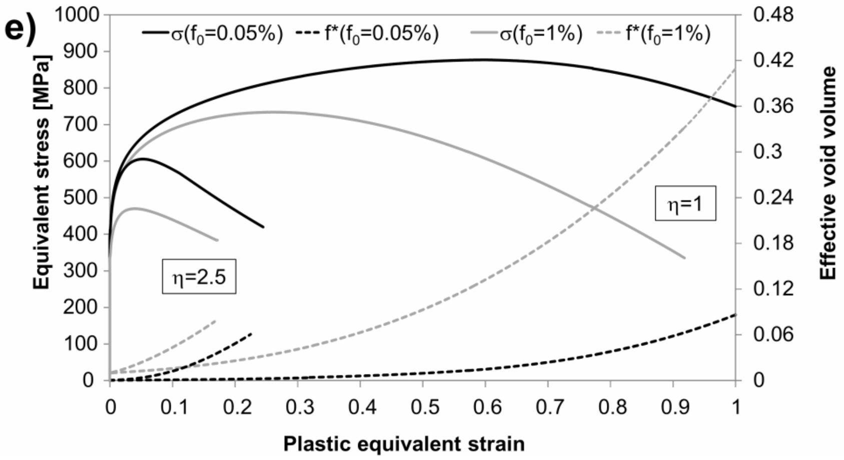
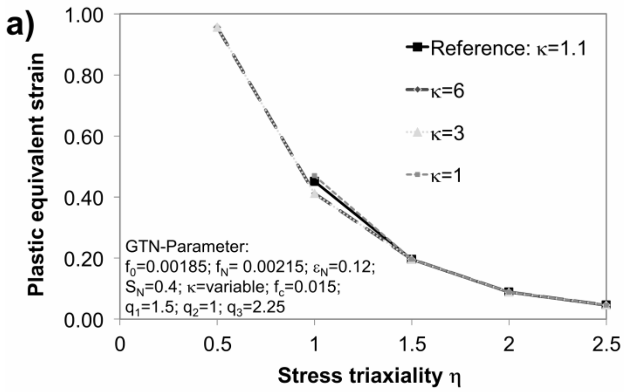
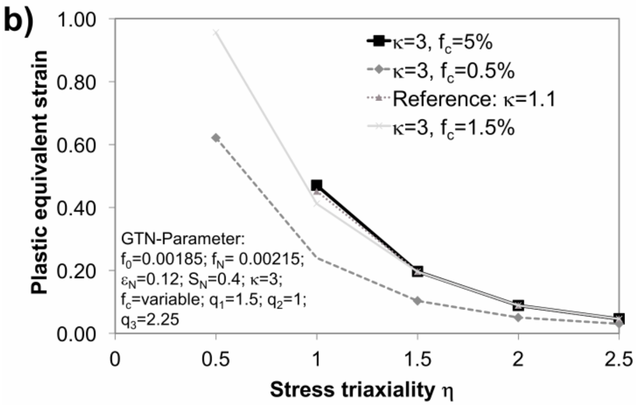


Figure 2. Damage curves under variation of a) f_0 b) f_N c) ε_N & d) S_N. Subfigure e) Equivalent stress and effective void volume as a function of the plastic equivalent strain under variation of f_0 for η=1 and η=2.5.

3.1.3. Influence of the void coalescence parameters f_c and κ

The void coalescence behaviour is implemented in the GTN model by an acceleration of void growth and nucleation. The critical void volume f_c determines the onset of acceleration, while the acceleration factor κ defines its magnitude. Therefore, f_c and κ have a crucial influence on the failure detection. Figure 3a displays the influence of κ on the damage curve. It is low with a maximum difference in critical strain of 6% at η=1. Figure 3c proves that there are significant differences in the corresponding stress-strain-curves. Since the strain at maximum stress is relevant for the derivation of the damage curve in this evaluation concept, κ only marginally impacts the damage curve. The value of f_c determines the onset of acceleration. With the currently calibrated low value of κ = 1.1 the influence of f_c on the damage curve is very small. It is therefore evaluated for an increased value of κ = 3. Figure 3b shows a significant influence of f_c on the damage curve for κ = 3, which is also reflected in the corresponding stress-strain-curves in Fig. 3c.





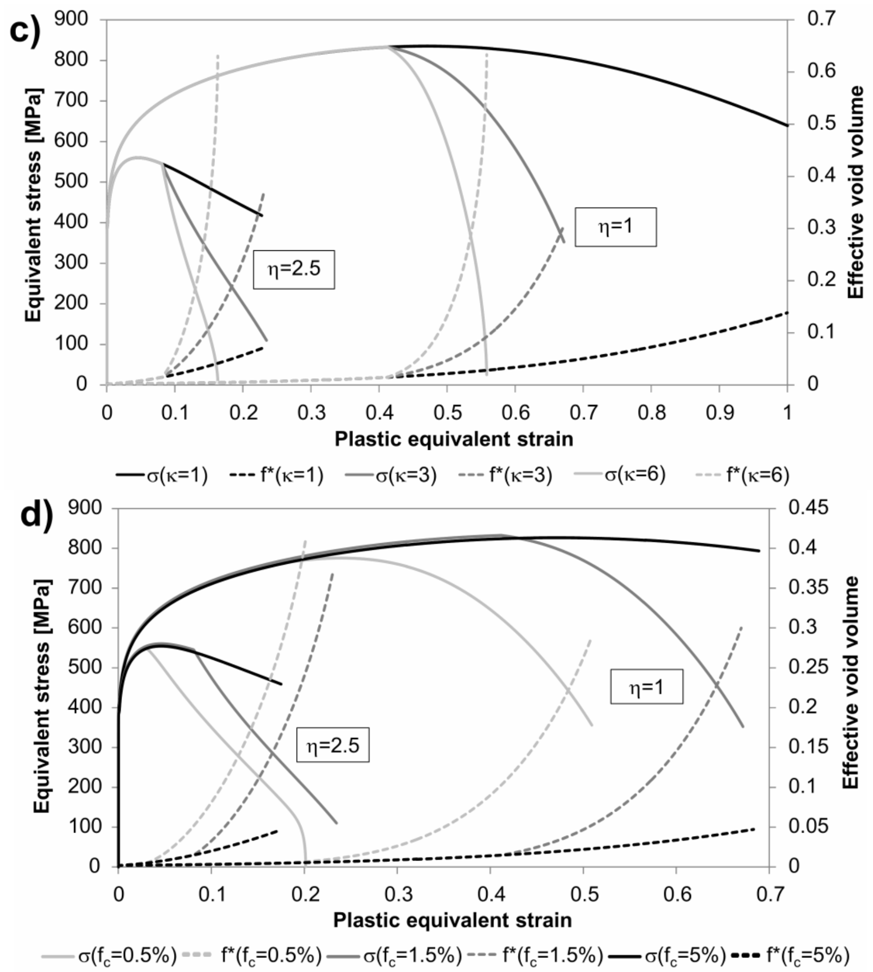


Figure 3. Damage curves under variation of a) κ b) f_c. Equivalent stress and effective void volume as a function of the plastic equivalent strain under variation of c) κ and d) f_c for η=1 and η=2.5.

3.1.4. Influence of the empirical fit parameters q_1 and q_2

The empirical fit parameters q_1 and q_2 have massive influence on the course of the damage curve, as can be seen in Fig. 4. The reason is that they directly change the shape of the yield surface. Contrary to most other parameters, the influence of q_2 is not decreasing with increasing triaxiality.

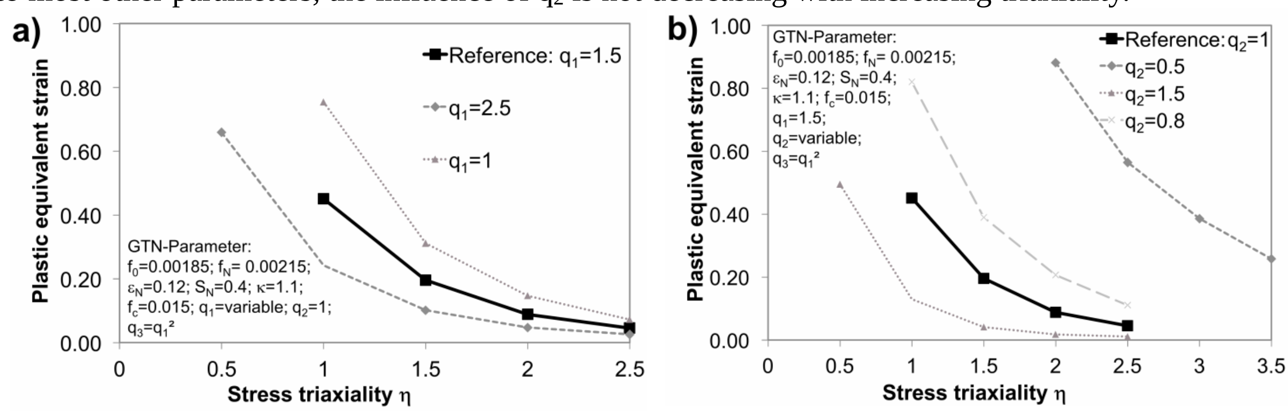


Figure 4. Damage curves under variation of a) q_1 and b) q_2.

3.1.5. Investigations on the uniqueness of the damage curve

The qualitative sensitivity analysis shows that the GTN parameter selection has a clear influence on the course of the damage curve. The impact of the individual parameters varies and their interaction is non-linear. Therefore, it is possible to determine several different parameter sets that yield the same result, the solution is not unique. Since the lower bound damage curve is calibrated at Charpy simulations in this methodology, two parameter sets are determined that compute a similar impact toughness and force-displacement-curve. In version A, f_N and S_N were increased to f_N=0.01 and S_N=2. In version B f_0 is decreased to f_0=0.001, while f_N is increased to f_N=0.015. Figure 5 shows the damage curves for these parameter sets. A good agreement can be found at higher triaxialities but the maximum difference of critical strain is 8% at η=1. The damage curve of version A is identical to the reference damage curve. The increased f_N should affect the damage curve, but due to the high S_N the nucleation of secondary voids is distributed over a broad strain interval so that the actual influence of f_N is diminished. Consequently, an identical damage curve is produced. Considering the micromechanical motivation of the GTN model this parameter selection is not sensible. Although the version B parameter set has a similar force-displacement curve, the influence of the important void parameters f_0 and f_N affects the course of the damage curve at low triaxialities.

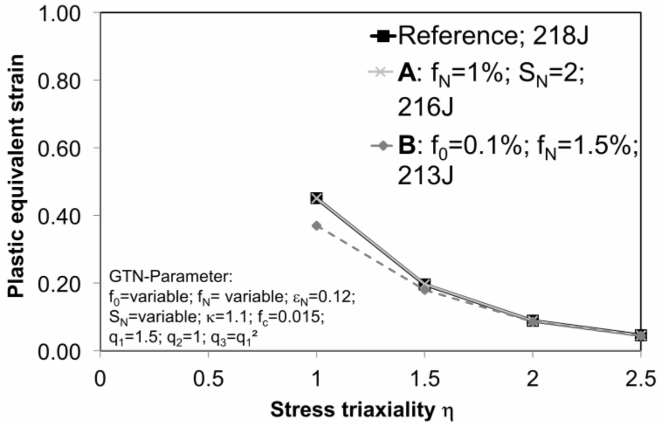


Figure 5. Damage curves for two parameter sets yielding a similar Charpy impact energy in simulation.

3.2. Discussion of the sensitivity analysis

The non-uniqueness of the GTN parameter selection may lead to identical damage curves resulting from different parameter sets if the interaction of individual parameters compensates their respective impacts. However, this is not always the case. Therefore, it is necessary to establish clear guidelines for the parameter derivation to ensure reproducible results. The guiding principle should be the micromechanical motivation of GTN. The basis for such a rule set is the performed sensitivity analysis. The impact and the consequences for the parameter derivation are discussed in the following for each variable.

Currently, the strain at maximum stress in the unit cell is considered as the crack initiation strain for the derivation of the damage curve. This enables a simple identification of the critical strain. This basic assumption needs to be considered during the GTN parameter calibration on tensile and fracture mechanics test. Consequently, the GTN parameter choice must ensure that in simulation of these samples the stress maximum of the failing element is correlated to the physical crack initiation measured in the experiment. An advantage of this criterion is that the mesh sensitivity of the results is reduced, since the mesh-dependence of the results begins with the onset of softening at the stress maximum [12].

The initial void volume fraction f_0 has a strong influence on the course of the damage curve. It can clearly be related to the microstructure of a material, since voids in many materials form at non-metallic inclusions at the onset of plastic deformation. f_0 has no direct interaction with other parameters but influences the whole computation from the beginning. Therefore, f_0 should be considered as the main parameter for the derivation of the lower bound damage curve. The micromechanically based motivation behind this procedure is that steel grades of low ductility often exhibit an increased amount of inclusion resulting in a poor internal cleanness. If f_0 is used as the main or even single parameter for the derivation of the lower bound criteria, its strong influence on the damage curve also facilitates the derivation of unique damage curves, since its effects cannot be compensated easily.

The volume fraction of potential secondary voids, f_N, also has a significant influence on the course of the damage curve. However, it is lower than the impact of f_0. For some materials, the nucleation sites for secondary voids can also be correlated to metallographic results, such as the carbide volume fraction. Even if this is not possible, the order of magnitude of f_N should be chosen in a micromechanically sensible range. In the nucleation function, f_N interacts with ε_N and S_N, which only have a low impact on the damage curve for common values of f_N. Their impact is increased proportionally with f_N. Therefore, if the nucleation parameters are modified, matching magnitudes should be selected to avoid non-uniqueness due to interactions. Alternatively, the modification could be restricted to f_N.

The coalescence parameters f_c and κ have a strong influence on the stress-strain-curve of the unit cell, since they determine onset and magnitude of the accelerated void growth. Consequently, there is also a relevant interaction of these parameters. If the critical strain f_c is reached after the maximum stress, the choice of κ and f_c has only little influence on the damage curve. This is more likely for high triaxialities. Since the maximum is correlated to crack initiation, κ should have a minimum value clearly larger than unity to enable a rapid failure of the element. This also reduces the influence of κ on the maximum stress point and consequently the damage curve. A further aspect is that the area beneath the stress-strain-curve is a measure for the dissipated energy. This is important for the parameter calibration of f_c and κ in tensile and fracture mechanics test. Different studies show the dependence of f_c on the stress triaxiality [3]. If possible, it is therefore advantageous to calibrate f_c such that the critical value is reached after the stress maximum of the critical element. If f_0 is modified for the derivation of the lower bound damage curve, it may therefore also be necessary to adapt f_c and κ.

The empirical fitting parameters q_i have massive influence on the course of the damage curve. Different studies show that a calibration of these parameters can improve the agreement between simulation and experiment [3]. However, considering the acceptance of the method and the reliability of the result it is better to keep the standard literature values, especially since they are able to represent the failure behaviour.

The definition of a fixed calibration scheme with respect to the considered experimental results is currently under research. Such a scheme can help to foster the acceptance of damage mechanics and may also be transferred to other applications than pressure vessels.

4. Application example of the lower bound damage curve in a pressure vessel simulation

The concept of the lower bound damage curve was applied to a pressure vessel simulation. It is loaded with increasing internal pressure. The lower bound damage curve is applied as the failure criterion. The resulting critical pressure is compared to the one defined by the design formulae of the current standard EN 13445 in the procedure “Design by Formulae” (DBF). Figure 6a shows the model, which could be reduced to a quarter of the vessel due to symmetry. The vessel has a mean diameter of 2600 mm and a wall thickness of 50 mm. The lug has a diameter of 631 mm and a wall thickness of 72.5 mm. P500Q is assumed as the material for the pressure vessel. The lower bound damage curve is derived according to the above explained concept. The parameters according to Eq. 4 are c_1= 0.94, c_2 = 1.76 and c_3=0.01. However, due to missing data, temperature and strain rate dependence are not yet considered. The results are therefore preliminary. Figure 6b shows the ductile damage criterion at the critical loading step, which highlights if the critical strain has been reached. The crack initiation takes place in the wall besides the lug. In this case, crack initiation happens in parallel with a plastic collapse.

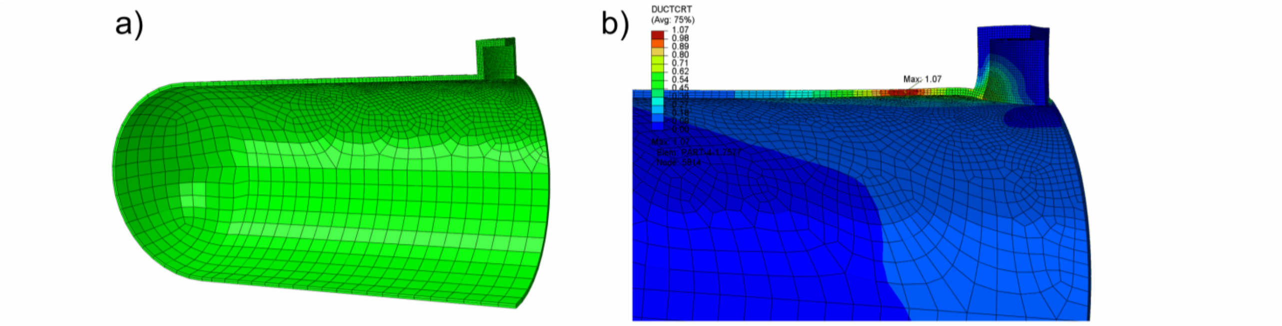


Figure 6. a) Quarter model of the pressure vessel b) Ductile crack initiation besides the lug

The internal pressure at failure is predicted to be 29.61 MPa. A design according to EN 13445 predicts a failure at a maximum pressure of 23.1 MPa. The damage curve concept can consequently be used to quantify unnecessary safety margins for high strength steels in pressure vessels.

5. Conclusions and Outlook

The nominal damage curve concept is a suitable approach to quantify unnecessary safety margins for high strength steels in pressure vessel design, which are included in the current European standard EN 13445. Its main advantage is that a failure prediction is possible under consideration of the nominal Charpy impact toughness by the application of the lower bound damage curve. Therefore, the materials ductility is considered in the design process. The application of this concept can help to derive more adequate safety factors for high strength steels. However, further research is necessary to ensure the safe application of this method. A sensitivity analysis shows that the course of the damage curve is influenced by the non-unique GTN parameter choice. Therefore, a calibration scheme with regard to the evaluated experimental results and considered nominal properties needs to be defined and is currently under research. Additionally, a modification of the applied GTN model towards a consideration of the third invariant of the stress tensor should be considered, since latest research shows that it has significant influence on the prediction of ductile fracture [2].

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