

Manuscript Details

Manuscript number	EFM_2019_187_R3
Title	Hydrogen informed Gurson model for hydrogen embrittlement simulation
Article type	Research Paper

Abstract

Hydrogen-microvoid interactions were studied via unit cell analyses with different hydrogen concentrations. The absolute failure strain decreases with hydrogen concentration, but the failure loci were found to follow the same trend dependent only on stress triaxiality, in other words, the effects of geometric constraint and hydrogen on failure are decoupled. Guided by the decoupling principle, a hydrogen informed Gurson model is proposed. This model is the first practical hydrogen embrittlement simulation tool based on the hydrogen enhanced localized plasticity (HELP) mechanism. It introduces only one additional hydrogen related parameter into the Gurson model and is able to capture hydrogen enhanced internal necking failure of microvoids with accuracy; its parameter calibration procedure is straightforward and cost efficient for engineering purpose.

Keywords	hydrogen enhanced localized plasticity; hydrogen-microvoid interaction; Gurson model; void growth
Taxonomy	Solid Mechanics, Computational Materials Science
Manuscript category	All other materials
Manuscript region of origin	Europe
Corresponding Author	zhiliang zhang
Corresponding Author's Institution	Norwegian University of Science and Technology
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Suggested reviewers	Xiaosheng Gao, Kim Verbeken, Lars Edvard Blystad Dæhli, Emilio Martínez Pañeda, Brian Nyvang Legarth

Submission Files Included in this PDF

File Name [File Type]

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Response to reviewer comments_R3.docx [Response to Reviewers]

HGurson_Rev3.pdf [Revised Manuscript with Changes Marked]

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Editor of VSI: Hydrogen Embrittlement
Engineering Fracture Mechanics

Prof. Zhiliang Zhang
Telephone no.: +4773592530

Dated:
2019-06-20

Our ref.:

Your letter dated:

Your ref.:

Dear Editor,

Attached please receive the revised manuscript titled "**Hydrogen informed Gurson model for hydrogen embrittlement simulation**" by Haiyang Yu, Jim Stian Olsen, Antonio Alvaro, Lijie Qiao, Jianying He and Zhiliang Zhang, submitted for consideration of publication in Engineering Fracture Mechanics VSI: Hydrogen Embrittlement.

Thank you for giving us another chance to revise the manuscript. We appreciate the suggestions given by the reviewers and revised the manuscript accordingly. Changes made to the manuscript are highlighted in red. We provide detailed response to the reviewers' comments in a separate document. Our response to the reviewers' comment are marked blue there. We also followed your instructions by listing the modifications directly in the response letter.

Sincerely yours,

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Hydrogen informed Gurson model for hydrogen embrittlement simulation

By H. Yu, J.S. Olsen, A. Alvaro, L. Qiao, J. He and Z. Zhang*

20 June 2019

We thank the reviewer for the comments. The manuscript has been revised according to the recommendations. **Changes made to the manuscript are highlighted in red.** We provide here detailed responses to the reviewer's comments. **Our responses to the reviewer's comment are marked blue in this document.**

Response to Reviewer's Reports:

Reviewer 1

The authors agree that the level of H softening is unrealistic. The new statement on pg. 13 to this effect is not, however, satisfactory because it is entirely non-quantitative. Given the absence (to my knowledge) of any observed macroscopic softening at H concentrations between 1-1000 ppm in most fcc and bcc materials (and in fact recent clear evidence of macroscopic hardening due to H at 1000 ppm levels in Ni, presumably due to H solute strengthening or H solute drag), the value $\psi = 0.9$ at $c_{OL}=1$ wppm is not only unrealistic, it is wildly so. And the authors then have a linear function so that the softening could be as large as 50% of the H-free value. The authors should therefore indicate how the magnitude of the effects here depends on the softening model. For instance, what is the result if $\psi = 0.99$ and $c_{OL}=1$ wppm (still very unrealistic)?

The linear hydrogen softening law and the lower bound of 50% are widely used in the literature [1-6]. Please note that this lower bound will not be reached during the simulation, as indicated in Fig.2b on Page 15.

On 13, we stated that "With less softening, the principle and the HGurson model still apply well, except that the absolute difference in the failure loci is less pronounced." In response to the reviewer's concern, we performed new simulations using $\psi = 0.99$ and $c_{L0}=1$ wppm and $\psi = 0.95$ and $c_{L0}=1$ wppm, and the results are plotted below in Fig.1 and Fig.2.

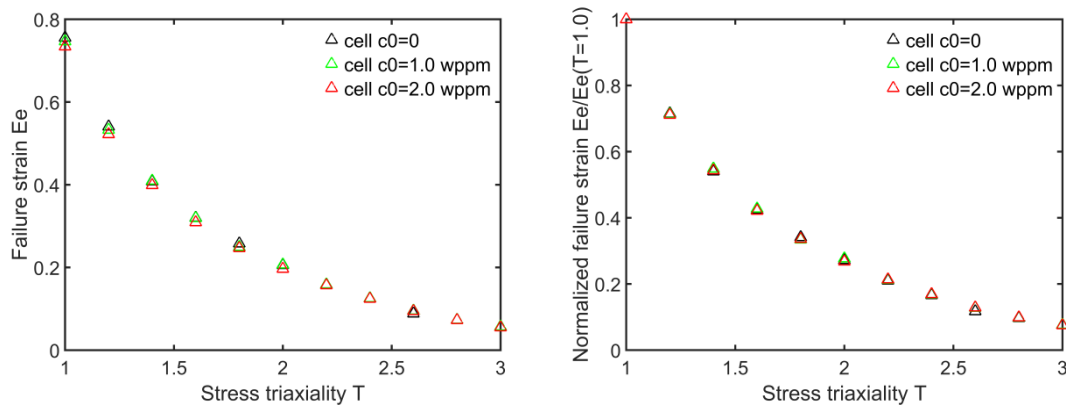


Fig.1 Failure loci obtained using $\psi = 0.99$ and $c_{L0}=1$ wppm. Left: the absolute failure loci; right: the normalized failure locus.

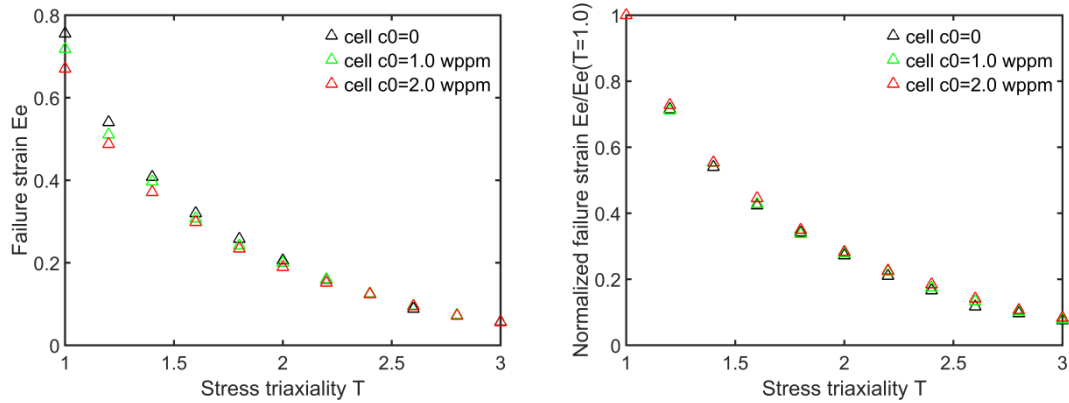


Fig.2 Failure loci obtained using $\psi = 0.95$ and $c_{L0}=1$ wppm. Left: the absolute failure loci; right: the normalized failure locus.

In these figures, the main conclusions of the paper, i.e. 1) hydrogen lowers failure strain and 2) the failure loci can be normalized (the decoupling principle), both hold, although the absolute difference is smaller. Since the HGurson model is developed based on these two basic assumptions, the model formulation will not be affected. In order to make a clear demonstration of the decoupling principle and model derivation procedure, we hope to keep the current parameters. As also indicated in our previous version of response, an even larger softening was adopted in [4], in order to make a clear demonstration of the void mechanism ($c_{L0}=1000$ wppm and $\psi=0.9$ and 0.8).

Following the reviewers suggestion, we included these two failure loci (the figures on the left in Fig.1 and Fig.2) in the appendix to support our statement made on Page 13:

“It should be noted that the assumed level of hydrogen softening is very large. This is for a larger contrast between hydrogen and original failure loci and for a better demonstration of the decoupling principle. With less softening, the principle and the HGurson model still apply well, except that the absolute difference in the failure loci is less pronounced. To give a sense of how the magnitude of the effect of hydrogen depends on the softening parameters, we include unit cell results with milder hydrogen softening, a 5% reduction and a 1% reduction with $c_L^0 = 1$ wppm , in Appendix A.”

The purpose of the discussion of lattice vs trapped H concentrations is not clear to me. The hypothetical constitutive law is based on total H, which itself makes no sense if the traps are, for instance, precipitates or precipitate interfaces, that have no connection to plasticity. On the other hand, dislocations are traps, and the H trapped at dislocations would presumably influence the plastic flow. So, the use of lattice vs. trapped H will always be ambiguous, and the authors present no useful information about this issue in any case. This could be deleted and the paper would be more clear.

The trap binding energy used in our simulations is typical for dislocation traps [7, 8]. The reviewer is right hydrogen trapped at dislocation can influence plastic flow, and this is exactly the reason why we can observe shearing failure at low triaxiality regime and necking failure in high triaxiality regime [4, 6, 7]. Suppose the

softening law is dependent only on lattice H instead of the total H, internal shearing will never be observed. Further, considering dislocations are mobile traps, the H trapped at dislocations should be regarded as mobile (“diffusible”) H, therefore, using the total H concentration is sensible.

The fact that the total H is used in the softening law and the dislocation trapped H can influence plastic flow is, however, not in conflict with the current work. It has been elaborated in our previous work [7] and also briefly mentioned in this work that dislocation trapped H can cause different failure modes (shearing vs necking), so this is evidence that trapped H makes contribution. However, when limited to the necking failure mode in high triaxiality regime, the trapped H makes a contribution very similar to the lattice H, since they both soften the material at the inter-ligament and promote internal necking failure. This was supported by the discussion in the first paragraph on Page 13.

Since this discussion is confusing to the reviewer, we have deleted it in the revision, following the reviewer's suggestion. We appreciate the suggestions of the reviewers, and we hope the reviewer is satisfied with our answers and modifications.

Reference

- [1] P. Sofronis, Y. Liang, N. Aravas, Hydrogen induced shear localization of the plastic flow in metals and alloys, *European Journal of Mechanics - A/Solids* 20(6) (2001) 857-872.
- [2] Y. Liang, P. Sofronis, N. Aravas, On the effect of hydrogen on plastic instabilities in metals, *Acta Materialia* 51(9) (2003) 2717-2730.
- [3] D.C. Ahn, P. Sofronis, R.H. Dodds Jr, On hydrogen-induced plastic flow localization during void growth and coalescence, *International Journal of Hydrogen Energy* 32(16) (2007) 3734-3742.
- [4] Y. Liang, D.C. Ahn, P. Sofronis, R.H. Dodds Jr, D. Bammann, Effect of hydrogen trapping on void growth and coalescence in metals and alloys, *Mechanics of Materials* 40(3) (2008) 115-132.
- [5] O. Barrera, A.C.F. Cocks, Computational modelling of hydrogen embrittlement in welded structures, *Philosophical Magazine* 93(20) (2013) 2680-2700.
- [6] S.M. Graham, X. Gao, T. Luo, C. Huang, Modeling the Effect of Hydrogen on Ductile Fracture, *Materials Performance and Characterization* 7(2) (2018).
- [7] H. Yu, J.S. Olsen, J. He, Z. Zhang, Hydrogen-microvoid interactions at continuum scale, *International Journal of Hydrogen Energy* 43(21) (2018) 10104-10128.
- [8] L. Jemblie, V. Olden, O.M. Akselsen, A coupled diffusion and cohesive zone modelling approach for numerically assessing hydrogen embrittlement of steel structures, *International Journal of Hydrogen Energy* 42(16) (2017) 11980-11995.

Hydrogen informed Gurson model for hydrogen embrittlement simulation

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Abstract

Hydrogen-microvoid interactions were studied via unit cell analyses with different hydrogen concentrations. The absolute failure strain decreases with hydrogen concentration, but the failure loci were found to follow the same trend dependent only on stress triaxiality, in other words, the effects of geometric constraint and hydrogen on failure are decoupled. Guided by the decoupling principle, a hydrogen informed Gurson model is proposed. This model is the first practical hydrogen embrittlement simulation tool based on the hydrogen enhanced localized plasticity (HELP) mechanism. It introduces only one additional hydrogen related parameter into the Gurson model and is able to capture hydrogen enhanced internal necking failure of microvoids with accuracy; its parameter calibration procedure is straightforward and cost efficient for engineering purpose.

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Keywords: Hydrogen enhanced localized plasticity, hydrogen-microvoid interaction, Gurson model, void growth

Nomenclature

\dot{f}	Void growth rate	c	Hydrogen concentration
η	Stress triaxiality	c_L	Lattice hydrogen concentration
\bar{V}_h	Partial molar volume of hydrogen	c_T	Trapped hydrogen concentration
σ_0	Initial yield stress without hydrogen	D_L	Hydrogen diffusion coefficient
σ_e	Equivalent stress	E	Young's modulus
σ_h	Hydrostatic stress	E_b	Trap binding energy
ε_0	Strain at yielding	f_0	Initial void volume fraction
ε_e	Effective strain	f_c	Critical void volume fraction
ε_f	Failure strain	R	Universal gas constant
ε_p	Plastic strain	T	Absolute temperature

1. Introduction

Continuum level hydrogen embrittlement (HE) simulation is one of the key aspects of failure assessment and control of engineering components exposed to hydrogen environment. A sound framework for this purpose consists of three basic ingredients, namely a plausible underlying HE mechanism, a

way to determine model inputs from experiments or lower scale simulations and eventually a continuum model applicable to various geometries and loading conditions. The underlying mechanism provides the physical foundation, the input calibration method serves as a bridge linking lower scale physics (often posed in a discrete manner) and continuum mechanics, and the model as the main carrier needs to be selected depending on the other two elements.

To date, there are two prevailing HE mechanisms, hydrogen enhanced decohesion (HEDE) and hydrogen enhanced localized plasticity (HELP). The HEDE mechanism assumes that dissolved hydrogen reduces the cohesive strength of the material lattice [1]; the HELP mechanism assumes that hydrogen facilitates dislocation activity thereby enhancing plasticity locally [2]. It is straightforward to see that HEDE is compatible with Griffith type fracture, so it is favorable for the simulation of HE which is usually accompanied by brittle-like fractography [3]. In fact, HEDE based continuum level HE simulation has been in progress for over a decade, thanks to cohesive zone modeling (CZM) which well represents the brittle fracture process [4]. By lowering the cohesive strength (fracture energy) of the cohesive interface with hydrogen content, hydrogen induced premature fracture in a brittle manner can be simulated. The determination of CZM parameters in the absence of hydrogen is out of the scope and not elaborated here. Hydrogen related inputs, i.e. hydrogen effects on CZM parameters, can be obtained based on atomistic calculations or experiments. Jiang and Carter [5] performed first principles calculations and found that the ideal fracture energy decreases almost linearly with increasing hydrogen coverage. This relation was then adopted by Serebrinsky et al. [6] and Olden et al. [7] in their hy-

drogen informed CZM (HCZM) simulations. Recently, Yu et al. [8] proposed a method to calibrate hydrogen dependent cohesive laws from tension tests. The HCZM approach is now rather mature and applied widely to engineering failure assessment [9, 10]. Following a similar pattern, the phase field approach was recently applied in HE simulation [11]. In spite of its popularity, HCZM has intrinsic deficiencies. While it “physically” represents the brittle failure caused by hydrogen, it cannot represent the ductile damage in the absence of hydrogen. Due to this inconsistency, it has to be admitted in the first place that HCZM is a phenomenological approach.

In contrast to the great popularity of the HELP mechanism, HELP based continuum model for hydrogen failure prediction is yet to be developed. There could be several reasons. First, the HELP mechanism claims more plasticity in the presence of hydrogen, so one may expect ductile fracture all the time, which doesn’t agree with the brittle-like HE fractography. Therefore, one could intuitively prefer HEDE to HELP as the underlying mechanism for continuum HE modeling. Secondly, unlike the HEDE case where the DFT results of hydrogen dependent cohesive law can be readily applied to the continuum level, the HELP mechanism, while verified by theoretical calculation using a pair of dislocations [2], cannot be quantitatively applied to the continuum level, since plasticity is the collective behavior of a large dislocation aggregate on which the hydrogen effect is still unclear. Finally, even if a phenomenological form for the HELP mechanism is temporarily assumed and implemented in unit cell analyses [12], the results are only qualitative ones due to the lack of a proper failure criterion. In short, a HELP based continuum model is still lacking because the underlying theory

seems inconsistent with reality and a bridge linking different scales is lacking.

The conditions for the development of HELP based continuum model has been largely improved recently. Yu et al. [13] proposed a failure criterion associated with hydrogen induced shear band forming in unit cell analysis, which allows failure to be detected at a very small void volume fraction at low stress triaxiality regime. That is, hydrogen induced premature failure with brittle-like fractography was predicted under the HELP mechanism solely. That work also demonstrated that more plasticity does not necessarily lead to higher ductility, it therefore removed the first obstacle for adopting HELP in a continuum model. Further, a hydrogen failure locus covering a wide range of stress triaxiality was established in that work, providing inputs for the continuum model. Meanwhile, it should be noted that the link between continuum scale and lower scales is still weak, since the HELP mechanism is implemented only conceptually using a phenomenological form in the cell analyses performed so far. Most recently, a hydrogen informed three dimensional discrete dislocation dynamics (HDDD) modeling framework was established [14], incorporating the elastic stress contribution from hydrogen as Eshelby inclusion [15] and hydrogen effects on dislocation mobility calibrated based on first principles calculations [16]. Global flow behavior was simulated with this method using a microcantilever geometry and hydrogen induced global softening, consistent with the HELP mechanism, was quantitatively captured at realistic bulk hydrogen concentrations. This framework addresses hydrogen influenced large dislocation aggregate property (plasticity) at microscopic scale and can therefore serve as an ideal bridge between the atomistic and continuum scales.

With the theoretical foundation and inter-scale bridge established, the construction of HELP based continuum model is now on the agenda. Although such model is still unavailable, lots of work on the mechanics of hydrogen induced failure due to HELP has been done, providing mechanistic insights. Sofronis et al. [17] introduced HELP to mechanical analyses by implementing a hydrogen softening law which prescribes the material yield stress as a decreasing function of hydrogen concentration. This method was then adopted by Ahn et al. [12], Liang et al. [18] and implemented in unit cell analyses. By zooming into a material point represented by a void containing representative material volume, the unit cell approach is an ideal tool to investigate material failure characterized by microvoid growth and coalescence process [19]. With hydrogen softening the matrix flow stress, material failure by void coalescence along the inter-ligament was found to occur earlier, i.e. hydrogen promoted internal necking failure. In [13], a hydrogen induced shearing failure mode was identified and quantified. This failure mode is observed in low stress traxiality regime and occurs with a much smaller void size compared to that in the internal necking mode, therefore, it captures the “embrittlement” feature of hydrogen caused failure. Most recently, Huang et al. [20] studied the effect of hydrogen under different Lode parameters with unit cell approach. These studies reveal the micromechanics of hydrogen caused premature failure under the HELP theory, with a merit that the basic failure process is consistently based on microvoid activity with or without hydrogen. Therefore, they open the door to a consistently micromechanics based continuum model which could be an alternative to the phenomenological HCZM framework for continuum HE modeling.

Given the background above, the Gurson model [21] seems to be an ideal starting point for a HELP based continuum model for HE simulation. This model describes the “average” flow behavior of a single void containing representative material volume (unit cell) during the development of the void (growth and coalescence), by ”smearing“the void throughout the unit cell and then viewing the smeared cell as a material point. Regarding void coalescence as the failure event, the Gurson model is able to predict failure if a critical void volume fraction is accordingly prescribed [22]. An alternative way to predict failure is to incorporate a physically based void coalescence criterion [23, 24, 25] to the Gurson model. During the past decades, a lot of improvement and adaption have been made on this model, breeding many different versions. In general, we refer to all the versions in this family as the Gurson model. Specifically, we based our discussion on the version developed by Tvergaard and Needleman [22] in this work. The Gurson model elegantly applies the mechanics happening locally in a unit cell to global specimen level and has achieved great success in engineering practice. It is also an ideal starting point for developing new microvoid mechanism based models, for which the modification of the Gurson model for shear [26] is a typical example. About one decade ago, it was realized that the ductile failure locus is dependent not only on stress triaxiality but also on the Lode parameter [27], and this was then studied extensively using unit cell approach [28, 29]. Inspired by the micromechanics revealed in cell analyses, Nahshon and Hutchinson [26] introduced a Lode parameter dependent term to the void growth rate term, making material failure shear sensitive. Essentially, this new model regards void volume fraction as a continuum damage parameter

which is made additionally dependent on Lode parameter. Therefore, this model is not as well physically based as the original Gurson model, nevertheless, it is still micromechanism inspired and is widely adopted in practice [30]. Similar treatment on the Gurson model is found in [31] and [32].

The present work discusses the possibility of using the Gurson model to convey hydrogen-microvoid interaction mechanisms to the continuum scale. Should this work, a micromechanics inspired HELP based continuum modeling tool for HE can be delivered. This potential model is referred to as the hydrogen informed Gurson (HGurson) model hereinafter. Starting from hydrogen-microvoid interactions, a possible form of HGurson model is proposed, together with a suitable parameter calibration procedure. At the moment, we don't aim to deliver a complete HGurson model ready for use, given the complexity in hydrogen assisted microvoid failure process. Instead, we elaborate the challenges in the development of such a model, propose solutions for some of them and leave the rest for future study. As a brief overview, the challenges/complexities include (but are not limited to): hydrogen trapping, change of failure mode in different stress triaxiality regime, inhomogenous material softening due to hydrogen redistribution and the form of hydrogen softening law. Being aware of all these complexities, we hereby limit our focus to a simple case with a linear softening law in high triaxiality regime, and a prototype HGurson model is presented.

2. Hydrogen-microvoid interactions

Hydrogen microvoid interactions are investigated via hydrogen diffusion coupled unit cell analyses [13]. J2 flow theory with isotropic hardening is

applied to describe the plastic flow in the matrix material

$$\sigma_f = \sigma_0(c) \left(1 + \frac{\varepsilon_p}{\varepsilon_0}\right)^n \quad (1)$$

where σ_f is the flow stress, $\sigma_0(c)$ the initial yield stress which is a function of the total hydrogen concentration c , ε_p the plastic strain and $\varepsilon_0 = \sigma_0/E$ the corresponding yield strain with E being the Young's modulus. To account for the HELP mechanism, the flow stress in the matrix material is assumed to decrease with hydrogen content. More specifically, the initial yield stress σ_0 is prescribed as a decreasing function of hydrogen concentration, for which the linear form [12] is most widely adopted

$$\sigma_0(c) = \begin{cases} [(\xi - 1)\frac{c}{c_L^0} + 1]\sigma_0 & \sigma_0(c) > \zeta\sigma_0 \\ \zeta\sigma_0 & \sigma_0(c) \leq \zeta\sigma_0 \end{cases} \quad (2)$$

where σ_0 is the initial yield stress with zero hydrogen concentration, $\xi\sigma_0$ the initial yield stress at the initial lattice hydrogen concentration c_L^0 and $\zeta\sigma_0$ the lowest possible value of the yield stress considering that hydrogen cannot cause the yield stress to vanish in reality.

The total hydrogen population consists of the lattice hydrogen residing at normal interstitial lattice sites and the trapped hydrogen residing at dislocation traps

$$c = c_L + c_T \quad (3)$$

where c_L is the lattice hydrogen concentration and c_T the trapped hydrogen

concentration. These two quantities can be further expressed as

$$c_L = \theta_L N_L \quad c_T = \theta_T N_T \quad (4)$$

where θ_L is the fraction of occupied interstitial lattice sites and N_L the lattice site density; similarly, θ_T is the fraction of occupied trapping sites and N_T the trapping site density.

Assuming steady state hydrogen distribution, the material flow stress is dependent on the hydrostatic stress field and the plastic strain field, which can be implemented to realize hydrogen coupled unit cell analysis [12]. Alternatively, transient hydrogen diffusion analysis can be directly coupled with unit cell analysis [13], which can be realized with the help of user subroutines in a commercial finite element software such as ABAQUS [33]. Under the limit of sufficient diffusion time, these approaches are equivalent, and the latter is adopted in this work. Transient hydrogen diffusion is governed by

$$\frac{\partial c_L}{\partial t} + \frac{\partial c_T}{\partial t} - \nabla \cdot (D_L \nabla c_L) + \nabla \cdot \left(\frac{D_L c_L \bar{V}_h}{RT} \nabla \sigma_h \right) = 0 \quad (5)$$

where D_L stands for the lattice diffusivity coefficient, \bar{V}_h the partial molar volume of hydrogen and σ_h the hydrostatic stress. An equilibrium exists between hydrogen in lattice sites and in trapping sites [34]

$$\frac{\theta_T}{1 - \theta_T} = \frac{\theta_L}{1 - \theta_L} K_T \quad (6)$$

where K_T is the trap equilibrium constant $K_T = \exp(-E_b/RT)$ with E_b being the trap binding energy, R the universal gas constant and T the absolute

temperature.

The unit cell method focuses on a single void behavior in a representative material volume with periodic boundary condition. It offers accurate control over loading path and is an ideal approach to construct material failure loci [35]. The failure locus is defined as a relation between the effective strain at failure ε_f and the geometric constraint. The level of geometric constraint can be characterized by stress triaxiality and Lode parameter [13]. In this work, the cylindrical unit cell [19] under proportional loading is employed, leading to an axisymmetric loading scenario where the Lode parameter remains constant $L \equiv -1.0$. In other words, 2D failure loci are concerned throughout this work. The effective strain of the unit cell is defined as [19]

$$\varepsilon_e = \frac{2}{3}|\varepsilon_3 - \varepsilon_1|, \quad (7)$$

where $\varepsilon_3 = \ln(L/L_0)$ and $\varepsilon_1 = \ln(R/R_0)$, with L and R being the current cell height and radius, respectively. And the level of constraint is characterized by stress triaxiality

$$\eta = \frac{\sigma_h}{\sigma_e}, \quad (8)$$

with σ_e being the equivalent stress.

With a similar approach, we studied the effect of hydrogen on material failure loci in a previous work [13] and a complicated picture was revealed. The effect was found to depend on hydrogen trap strength as well as stress triaxiality. With weak trapping, failure occurred in internal necking mode over the entire range of triaxiality, and hydrogen promoted this failure mode. With strong trapping, hydrogen induced the formation of a shear band in

the low triaxiality regime, giving rise to a new internal shearing failure mode. This adds complexity to the development of the HGurson model. Ultimately, a successful HGurson model is expected to reproduce the hydrogen failure loci, capturing all the complexities involving trapping strength dependency and different failure modes. This work as a starting point, is devoted only to capturing hydrogen promoted internal necking failure mode, which is the first issue that should be addressed in model development. In other words, we limit our focus here to the medium and high stress triaxiality regime $\eta > 1.0$.

Hydrogen diffusion coupled unit cell analysis describes the mechanical process in a representative material volume, which is viewed as a material point at the specimen level. Therefore, HGurson model is essentially a homogenized description of hydrogen-microvoid interactions at material points. In this sense, the cell analyses can be regarded as “virtual experiments” that can be used as reference to calibrate and validate the HGurson model. Such “virtual experiments” need to be performed with various hydrogen concentrations. In all the cell analyses here, the Young’s modulus is $E = 2 \times 10^5 \text{MPa}$, the initial yield stress of the material is $\sigma_0 = 400 \text{MPa}$, and the strain hardening exponent is $n = 0.1$. The initial void volume fraction of the unit cell is $f_0 = 0.0013$ in all simulations. The linear hydrogen softening law in [Equation 2](#) is adopted with $\xi = 0.9$ and $\zeta = 0.5$. Lattice hydrogen properties relevant to steel are adopted: the lattice site density is taken as $N_L = 8.74 \times 10^{19}$ sites/ mm^3 , the partial molar volume of hydrogen as $\bar{V}_h = 2 \times 10^3 \text{mm}^3/\text{mol}$ and lattice diffusion coefficient as $D_L = 2.5 \times 10^{-11} \text{m}^2/\text{s}$. The same trapping parameters as in [\[13\]](#) representing a strong trapping scenario are adopted. The reference hydrogen concentration ([Equation 2](#)) at which a 10% reduc-

tion in yield stress is observed is assumed to be $c_L^0 = 1.0\text{wppm}$. The loading rate during simulation is sufficiently low so that steady state hydrogen distribution is guaranteed. **It should be noted that the assumed level of hydrogen softening is very large. This is for a larger contrast between hydrogen and original failure loci and for a better demonstration of the decoupling principle. With less softening, the principle and the HGurson model still apply well, except that the absolute difference in the failure loci is less pronounced. To give a sense of how the magnitude of the effect of hydrogen depends on the softening parameters, we include unit cell results with milder hydrogen softening, a 5% reduction and a 1% reduction with $c_L^0 = 1.0\text{wppm}$, in [Appendix A](#).**

Four cases with different initial uniform hydrogen concentrations $c_0 = 0.5, 1.0, 1.5, 2.0\text{wppm}$ and a hydrogen free case $c_0 = 0$ are investigated. Unit cell analyses are performed under fixed stress triaxiality ranging from $\eta = 1.0$ to $\eta = 3.0$ with an interval of 0.2. Over this range, only hydrogen promoted internal necking failure is observed. The failure loci are constructed for each hydrogen concentration.

The results of hydrogen coupled unit cell analyses, quantified as failure loci, are presented in [Fig. 1](#). Internal necking failure is observed over the entire range of triaxiality in all cases, and the failure strain decreases with the increase of hydrogen concentration.

Before establishing a model to capture these failure loci, the mechanism of hydrogen promoted internal necking failure needs to be analyzed. An intuitive impression is that hydrogen induced softening of the matrix material accounts for the early failure, since the initial yielding stress lowers

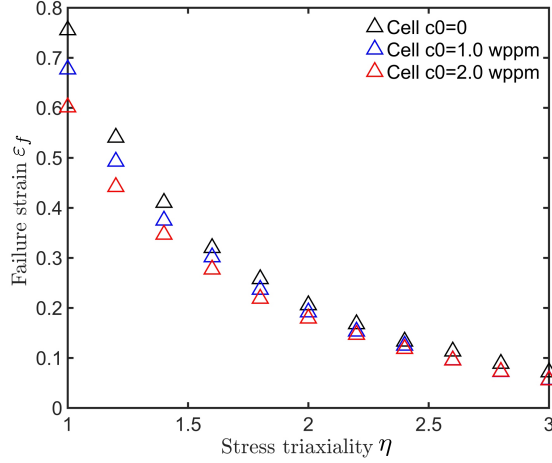


Fig. 1 The failure loci obtained by hydrogen diffusion coupled unit cell analyses, with and without hydrogen.

as c_0 increases. Looking into the hydrogen distribution contour during the loading process, another possible reason is spotted. Due to the pressure and plastic strain dependent nature of hydrogen redistribution, higher hydrogen concentration is built up at the inter-ligament region, which in turn leads to non-uniform hydrogen softening across the unit cell, as shown in Fig. 2. This could also be a rationale for the premature failure. To distinguish between these causes, we refer to the former rationale as hydrogen caused uniform softening and the latter as hydrogen caused non-uniform softening.

To probe the actual cause, an artificial case where the initial yield stress of the matrix material is decreased uniformly by 50% (the lower bound of hydrogen softening) was simulated. The void growth curves in this case and in the realistic cases with and without hydrogen are plotted in Fig. 3. Clearly, hydrogen caused uniform softening in the matrix material contributes little to the acceleration in void growth and premature failure, indicating hydrogen

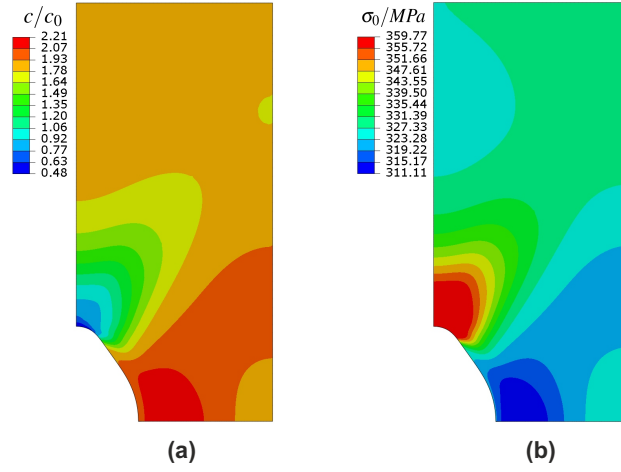


Fig. 2 (a) The distribution of hydrogen concentration and (b) the initial yield stress contours at an effective strain $\epsilon_e = 0.5$ and stress triaxiality $\eta = 1.0$, obtained with hydrogen $c_0 = 1.0$ wppm.

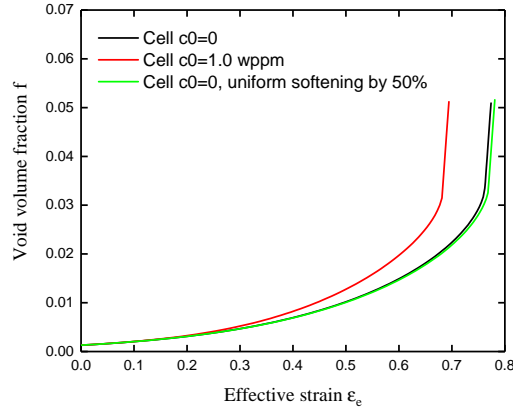


Fig. 3 Void growth curves obtained via unit cell analyses at stress triaxiality $\eta = 1.0$, including the hydrogen free case, a hydrogen case and an artificial case where no hydrogen is present but the entire matrix material is uniformly softened by 50%.

caused non-uniform softening plays a dominant role. This provides important reference for subsequent model development.

3. HGurson formulation

Coming back to the failure loci in Fig. 1, it is observed that they generally follow a same trend, which is clearly demonstrated by applying a normalization scheme as shown in Fig. 4(a). The scheme was performed by normalizing

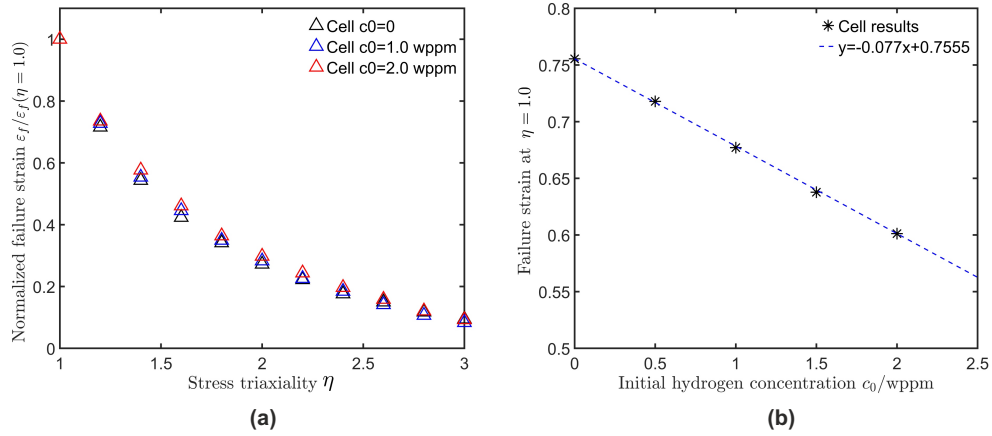


Fig. 4 (a) The normalized failure loci; the failure loci approximately collapse into one curve upon normalization. (b) The value used for normalization versus initial hydrogen concentration, which shows a linear relation.

the failure strain values on each failure locus by the value corresponding to $\eta = 1.0$ on the same locus. After normalization, all the failure loci, including the hydrogen free failure locus, collapsed into one curve, verifying that they have the same triaxiality dependence, so the presence of hydrogen just scales the absolute value of a specific locus. In other words, it indicates the failure strain $\varepsilon_f(\eta, c)$ which is a function of stress triaxiality and hydrogen concentration can be expressed in a decoupled form

$$\varepsilon_f(\eta, c) = f(\eta) \cdot h(c) \quad (9)$$

with $f(\eta)$ determined in Fig. 4(a) and $h(c)$ in Fig. 4(b). It should be noted that $h(c)$ is a “hydrogen scaling” function that is calibrated from the “virtual experiments” instead of a fitting parameter. The decoupling phenomenon has been observed in the case without trapping as well as in the current case. It may be attributed to the fact that the same failure mechanism, i.e. hydrogen induced local softening and the similar softening pattern, e.g. Fig. 2(b), apply at different hydrogen concentrations. This decoupling principle holds true as long as the hydrogen induced local softening occurs at the inter-ligament, which is the case in the high triaxiality regime concerned here. In the low triaxiality regime where internal shearing failure is observed [13], this principle needs to be verified separately. The fact that the hydrogen free case also follows this rule suggests that we can start from a hydrogen free mechanical model and then incorporate the scaling due to hydrogen to capture the hydrogen failure loci. To predict failure of microvoids without hydrogen, the Gurson model is a perfect candidate.

3.1. Gurson model

The Gurson model [36] is a popular approach to describing failure in porous materials. In 1975, Gurson [36] studied the macroscopic plastic flow of a long circular cylindrical void in a matrix of rigid-plastic von Mises material. By utilizing an approximate velocity field and appropriate boundary values at the outer and void surface, an upper bound yield function was derived

$$\phi(\boldsymbol{\sigma}, \bar{\sigma}, f) = \left(\frac{\sigma_e}{\bar{\sigma}}\right)^2 + 2q_1 f \cosh\left(\frac{q_2 \sigma_m}{2\bar{\sigma}}\right) - 1 - q_3 f^2 = 0 \quad (10)$$

where $\boldsymbol{\sigma}$ is the stress tensor and f the void volume fraction; σ_e is the macroscopic equivalent stress and σ_m the mean stress. q_1 , q_2 and $q_3 = q_1^2$ are the parameters introduced by Tvergaard and Needleman [22] in order to enhance the fitting capacity. This modified version is usually referred to as the GTN model [37], and the original Gurson model is retrieved by setting q_1 , q_2 and q_3 to 1. In this model, the porous material is represented by a void free continuum, and the microvoids are “smeared” across the continuum.

When loaded, the void volume fraction f of the material increases due to microvoid growth, and the yield surface is modified following Equation 10. The rate of void volume change \dot{f} , i.e. void growth rate is derived from the mass conservation condition in the matrix

$$\dot{f} = (1 - f)D_{kk}^P \quad (11)$$

where D_{kk}^P is the volumetric strain rate. It is assumed that failure initiates when the void volume fraction reaches a critical value $f = f_c$. Therefore, f could be regarded as a damage parameter with a sound micromechanical basis.

The GTN version is employed here to capture the microvoid failure locus in the absence of hydrogen. Consistent with the unit cell analyses, the material initially possesses a void volume fraction $f_0 = 0.0013$ and void nucleation is not taken into account. The same mechanical properties for the unit cell matrix are assigned to the Gurson matrix. Unit cell analyses show that the critical void volume fraction at failure initiation is around 0.03, therefore, $f_c = 0.03$ is adopted in the Gurson model. A single element model assigned with Gurson material is employed, in order to verify the predictions against

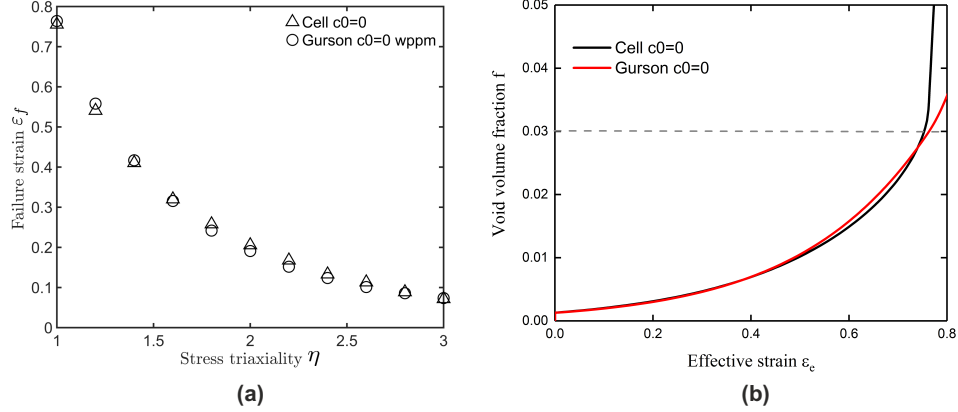


Fig. 5 Using the Gurson model to capture (a) hydrogen free failure locus and (b) void growth in the case with stress triaxiality $\eta = 1.0$.

the cell results. This element corresponds to the material point represented by the unit cell in [section 2](#). The same loading conditions, e.g. fixed stress triaxiality, are applied to the single element model as to the unit cell. The GTN fitting parameters are selected as $q_1 = 1.3$, $q_2 = 1.0$, $q_3 = 1.69$, which yields the best prediction of the hydrogen free failure locus. The Gurson model predictions of unit cell failure locus and void growth in the case of $\eta = 1.0$ are presented in [Fig. 5](#). Good agreement between the model prediction and the cell results are achieved.

3.2. HGurson model

Following the decoupling principle revealed in the previous section, we now proceed to incorporate the effect of hydrogen into the Gurson model established above. Since the material point is represented by only one element in the HGurson model, hydrogen redistribution observed in the unit cell analyses cannot be directly captured. Therefore, the hydrogen concen-

tration that is passed to the model has to be the initial uniform hydrogen concentration applied to the unit cell: again, the entire hydrogen-microvoid interactions, including hydrogen redistribution and plasticity localization are captured in a homogenized manner by the HGurson model. Recall that it is the hydrogen caused non-uniform softening that is dominant in the premature failure, but this cannot be reflected directly in the single element model. Looking at the derivation of the original Gurson model, we face the same dilemma: the Gurson model was derived assuming an isotropic matrix with uniform mechanical property, therefore, hydrogen can only soften the entire volume, in other words, there is no way to implement non-uniform hydrogen softening, if we wish to rigorously keep the original formulation of the Gurson model.

To demonstrate the deficiency of considering only the hydrogen caused uniform softening effect in HGurson model, we use a simple artificial case where the single element Gurson model is simulated at $\eta = 1.0$ and the initial yield stress of the matrix material is decreased by 50% uniformly. This artificial HGurson case corresponds to the artificial cell case in [Fig. 3](#). The void growth curve has been included in [Fig. 8\(a\)](#). Clearly, directly implementing uniform softening to the Gurson model has little influence on void growth and therefore does not help capture the hydrogen failure loci.

To account for the hydrogen caused non-uniform softening effect in the HGurson model, the rigorous way is to reformulate the original Gurson model to consider a local softening regime in the void ligament. The solution will be extremely difficult, if not impossible, and it requires quantitative description of hydrogen induced non-uniform softening when it comes to the HGurson

model, which induces further complexity. An alternative way is to view the Gurson model as a damage model and the void volume fraction f a damage parameter, so that the premature failure can be attributed to the hydrogen promoted accumulation of damage. The latter is adopted in this work, inspired by the practice in [26] which introduced the influence of external shearing to the Gurson model.

The strategy is therefore to let hydrogen accelerate damage accumulation in the Gurson model, and the acceleration should be dependent on hydrogen concentration. For this purpose, the void growth rate \dot{f} is made additionally dependent on the initial hydrogen concentration c_0 applied to the material point. It should be noted that c_0 is referred to as the initial concentration in the sense that it prescribes the hydrogen condition at the beginning of hydrogen-microvoid interaction, at each material point and for a given time step in HGurson simulation. At the specimen level, c_0 should correspond to the transient hydrogen concentration at materials points instead of the global concentration initially applied to the whole specimen. In the lack of further information on hydrogen accelerated damage accumulation, the linear scaling function stands as a natural option [26]

$$\dot{f}(c_0) = \dot{f}_0 \cdot k_H(c_0) = (1 - f)D_{kk}^P \cdot k_H(c_0) \quad (12)$$

As to be shown later, this function can yield satisfactory failure prediction. In this formulation, the void growth rate in the presence of hydrogen is simply the hydrogen free void growth rate $\dot{f}_0 = \dot{f}(c_0 = 0)$ multiplied by a scaler as a function of hydrogen concentration at the material point. In the case of the single element model, since the initial hydrogen concentration is constant,

this scaler is a constant. Therefore, this scaler function can be calibrated via comparison between the single element model and unit cell results.

Applying [Equation 12](#) and keeping all the other parameters unchanged, the void growth rate will be accelerated. However, it is not easy to evaluate the acceleration analytically, since the volumetric strain rate D_{kk}^P in this expression will also be increased due to the modification. Assuming D_{kk}^P remains constant throughout the simulation, we have

$$\int_0^{\varepsilon_{f0}} \dot{f}_0 d\varepsilon = f_c \quad (13)$$

$$k_H(c_0) \cdot \int_0^{\varepsilon_f(c_0)} \dot{f}_0 d\varepsilon = f_c \quad (14)$$

where ε_{f0} denotes the hydrogen free failure strain. [Equation 14](#) indicates the hydrogen failure strain $\varepsilon_f(c_0)$ is equivalent to the strain value corresponding to the void volume fraction $f_c/k_H(c_0)$ in the hydrogen free case. In the simplest scenario where \dot{f}_0 is constant, i.e. the void growth curve is linear, we have

$$k_H(c_0) = \frac{\varepsilon_{f0}}{\varepsilon_f(c_0)} \quad (15)$$

In practice, however, the void growth curve is concave up as shown in [Fig. 6](#). In this figure, the actual failure strains are $\varepsilon_f = 0.682$ and $\varepsilon_f = 0.764$ in the $c_0 = 1.0wppm$ and $c_0 = 0$ cases, respectively. Due to the linear void growth assumption, the scaler is determined as $k_H = 1.16$, yielding a prediction of $\varepsilon_f = 0.733$, $\approx 7.5\%$ higher than the actual value. Therefore, the linear void growth assumption leads to overestimation. Meanwhile, it is noted that the

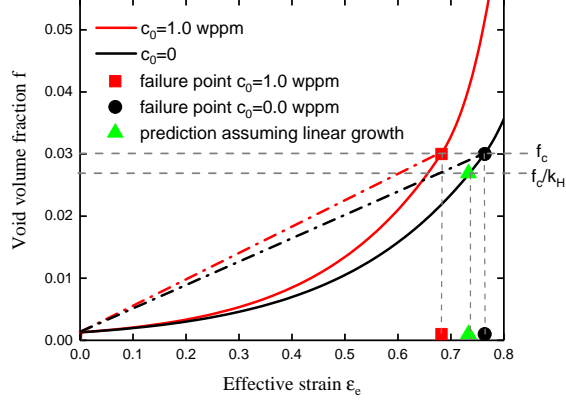


Fig. 6 The prediction of hydrogen failure point using Equation 14 and assuming linear void growth. The solid lines represent the actual void growth curves extracted from HGurson simulations, and the dashed dotted lines represent the assumed linear void growth line. k_H is determined as $k_H = \frac{\varepsilon_{f0}}{\varepsilon_f(c_0=1.0wppm)}$.

discussion above is based on the assumption that D_{kk}^P remains constant after implementing Equation 12. As a matter of fact, D_{kk}^P is found to increase in the simulation with hydrogen, scaled up approximately by a factor of $\alpha \cdot \varepsilon_e$, with $\alpha > 1.0$ roughly being a constant and ε_e the effective strain. This implies the failure strain predicted with Equation 14 and Equation 15 in practice will be smaller than that estimated in Fig. 6. In other words, the overestimation eventually will be less than 7.5%, making the prediction rather satisfactory.

Going back to Fig. 4 and Equation 9, we now have

$$k_H(c_0) = \frac{\varepsilon_f(\eta, 0)}{\varepsilon_f(\eta, c_0)} = \frac{h(0)}{h(c_0)}, \quad (16)$$

so the parameter k_H is a function of c_0 and independent of stress triaxiality.

k_H as a function of c_0 can then be calibrated based on Fig. 4(b)

$$k_H(c_0) = 0.16c_0 + 1.0. \quad (17)$$

It should be emphasized that this function is obtained via calibration of the unit cell failure loci following the decoupling principle, rather than out of pure fitting.

The HGurson model is established by implementing Equation 12 and Equation 17. This model is then implemented via user defined material subroutine UMAT in ABAQUS [33], using the explicit consistent tangent modulus method [38, 39, 40]. The hydrogen failure loci predicted by the single element HGurson model for the cases $c_0 = 1.0wppm$ and $c_0 = 2.0wppm$ are shown in Fig. 7. Satisfactory agreement between the HGurson predictions

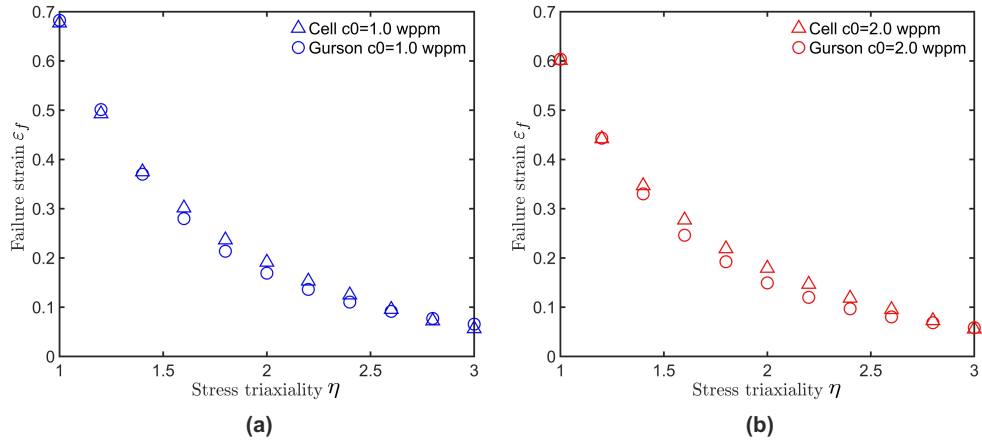


Fig. 7 Single element HGurson model prediction of hydrogen failure loci for (a) $c_0 = 1.0wppm$ and (b) $c_0 = 2.0wppm$.

and the unit cell results is achieved. Except for the failure strain, the void growth curve and stress-strain relation are also captured with good accuracy,

which is verified by comparing the HGurson and unit cell results with $\eta = 1.0$ and $c_0 = 1.0\text{wppm}$, as shown in Fig. 8.

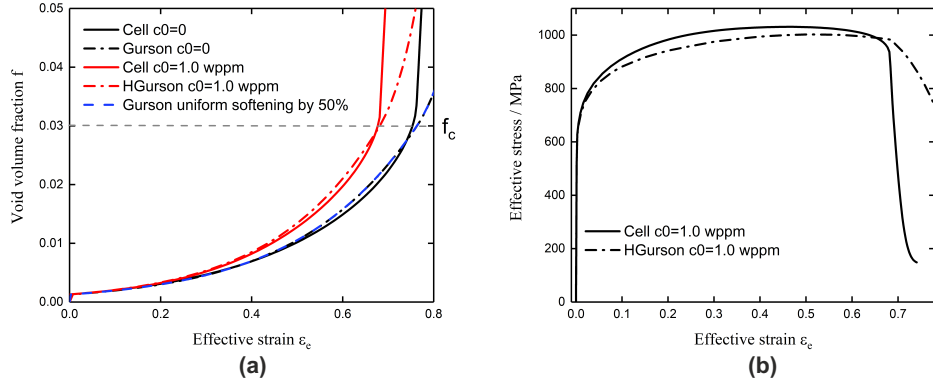


Fig. 8 The HGurson model prediction of (a) void growth curve and (b) effective stress-strain relation for the case with $\eta = 1.0$ and $c_0 = 1.0\text{wppm}$. The void growth curves without hydrogen and a (artificial) void growth curve obtained by softening the original Gurson model uniformly are also included in (a).

So far, an HGurson model accounting for hydrogen enhanced internal necking failure has been delivered. This model reproduces the “virtual experimental” results obtained via hydrogen diffusion coupled unit cell analyses. For a given material, this model keeps all the hydrogen free material properties calibrated for the Gurson model and introduces only one additional hydrogen acceleration of void (damage) growth term $k_H(c_0)$, which is dependent only on hydrogen concentration c_0 . In real life, the void behaviour is more complicated, accompanied by rotation and shape change. These will inevitably affect model parameters, such as the critical void volume fraction f_c and the q parameters in the GTN version. To consider the hydrogen dependence of these parameters, more parameters and assumptions have to be included and additional calibrations are required, rendering the model redun-

dant. Following the decoupling principle regarding the effect of hydrogen, we keep all the Gurson parameters unaffected by hydrogen, once they are determined in the hydrogen free case. This yields a clean HGurson model with good accuracy. Similar practice is found in the shear modified Gurson model [26]. As noted before, c_0 is the initial uniform hydrogen concentration in the single element model, but it will be the real time hydrogen concentration at material points in specimen level simulations. The application of Equation 2 will cause softening to plastic flow, which will occur mainly at the failure process zone where a high concentration of hydrogen is built up. In most part of the specimen, hydrogen concentration will remain low and therefore the global loading curve is not expected to be severely softened.

The HGurson model is of practical value for engineering failure assessment to which material failure locus is critical. To calibrate a failure locus, the conventional way is to design test specimens with various geometries representing a range of stress triaxialities; the specimens are then loaded to failure so that the relation between failure strain and stress triaxiality can be obtained. For hydrogen failure assessment, the whole procedure has to be repeated under different hydrogen concentrations, in order to construct hydrogen failure loci as shown in Fig. 1, which increases the workload by several times. Inspired by the decoupling principle revealed in Fig. 4, the calibration procedure for the HGurson model and hence for failure loci can be significantly simplified:

- (I) A series of mechanical tests with different geometries (stress triaxialities) in the absence of hydrogen need to be performed on a given material, yielding hydrogen free Gurson model parameters (hydrogen

free failure locus), e.g. [41].

- (II) Hydrogen charged mechanical tests need to be performed using any (one) geometry at several hydrogen concentrations to produce a hydrogen degradation curve similar to that in Fig. 4(b), and the hydrogen related term $k_H(c_0)$ (Equation 17) can then be determined.

In this procedure, different geometries need to be tested only in step (I), which is the necessary cost for material calibration in the absence of hydrogen. In step (II), utilizing the decoupling concept, only one specimen geometry is needed and only a couple of hydrogen concentrations need to be tested. Therefore, this HGurson model calibration procedure is cost efficient for engineering purpose.

4. Summary

A hydrogen informed Gurson model for hydrogen enhanced internal necking failure in high stress triaxiality regime was established in this work, as the first step towards a practical hydrogen embrittlement simulation tool based on the HELP mechanism.

Using hydrogen diffusion coupled unit cell analyses as “virtual experiments”, hydrogen enhanced internal necking failure loci were constructed at various concentrations and an important conclusion in hydrogen-microvoid interactions, i.e. the decoupling principle, was drawn. The hydrogen failure strain was shown to be a decreasing function of stress triaxiality and hydrogen concentration, and more importantly, the effects of these two factors were found to be decoupled. Further investigation demonstrated that hydrogen caused non-uniform softening of the unit cell matrix is the dominant factor

in hydrogen enhanced internal necking failure. These conclusions hold for a wide range of hydrogen trapping strength, as far as internal necking failure is concerned.

The HGurson model was proposed based these findings. Inspired by the decoupling concept, this model uses the Gurson model which accurately captures the hydrogen free microvoid process as the basis and introduces only one hydrogen related term to accelerate damage accumulation. Due to the clean formulation and the easy calibration of the hydrogen related term, the proposed model is user friendly and cost efficient for engineering practice. Good agreement between the HGurson model predictions and the “virtual experimental” results were achieved.

The HGurson model derivation was demonstrated using a strong hydrogen trapping case, since it gives pronounced hydrogen degradation in failure strain. In fact, we also studied the case with no hydrogen trapping and found that the model possesses the same form and follows the same derivation procedure. Therefore, this HGurson model is expected to apply to various hydrogen trapping strengths as far as internal necking failure mode is concerned.

This work concerns only hydrogen enhanced internal necking failure and is just the first step towards a HELP mechanism based hydrogen embrittlement simulation tool. To deliver a complete model applicable to the entire range of stress triaxiality, hydrogen induced internal shearing should also be addressed, which will be our next step.

Acknowledgements

The financial support from Aker Solutions and NTNU via the Integrity of Ni-Alloys for Subsea Applications (INASA) project is greatly acknowledged. We also want to thank the Research Council of Norway for funding through the Hydrogen-induced degradation of offshore steels in ageing infrastructure - models for prevention and prediction (HIPP). Contract No. 234130/E30.

Appendix A. Failure loci under milder hydrogen softening

In order to give a sense of how the magnitude of the effect of hydrogen depends on the softening parameters, we present the failure loci obtained using $\xi = 0.95, c_L^0 = 1.0\text{wppm}$ and $\xi = 0.99, c_L^0 = 1.0\text{wppm}$ (Equation 2). With milder hydrogen softening, the decrease in failure strain due to hy-

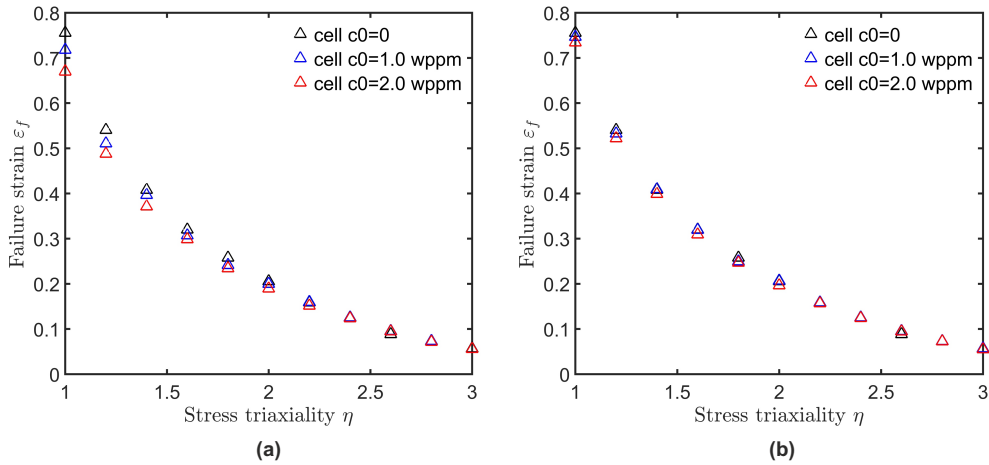


Fig. A.9 Failure loci obtained using unit cell analyses with milder hydrogen softening: (a) $\xi = 0.95, c_L^0 = 1.0\text{wppm}$ and (b) $\xi = 0.99, c_L^0 = 1.0\text{wppm}$.

drogen becomes smaller. However, the shape of failure loci are the same as that in Fig. 1; it has been verified that the decoupling principle, e.g. Fig. 4

and Equation 9 still holds. Therefore, the HGurson model formulation also applies in these cases with milder hydrogen softening.

References

- [1] R. A. Oriani, A mechanistic theory of hydrogen embrittlement of steels, *Berichte der Bunsengesellschaft für physikalische Chemie* 76 (1972) 848–857.
- [2] H. K. Birnbaum, P. Sofronis, Hydrogen-enhanced localized plasticity mechanism for hydrogen-related fracture, *Materials Science and Engineering: A* 176 (1994) 191–202.
- [3] H. Yu, Modelling and assessment of hydrogen embrittlement in steels and nickel alloys, PhD Diss, Norwegian University of Science and Technology (2003).
- [4] H. Khoramishad, J. Akbardoost, M. Ayatollahi, Size effects on parameters of cohesive zone model in mode I fracture of limestone, *International Journal of Damage Mechanics* 23 (2014) 588–605.
- [5] D. E. Jiang, E. A. Carter, First principles assessment of ideal fracture energies of materials with mobile impurities: implications for hydrogen embrittlement of metals, *Corrosion Reviews* 52 (2004) 4801–4807.
- [6] S. Serebrinsky, E. A. Carter, M. Ortiz, A quantum-mechanically informed continuum model of hydrogen embrittlement, *Journal of the Mechanics and Physics of Solids* 52 (2004) 2403–2430.

- [7] V. Olden, C. Thaulow, R. Johnsen, E. stby, T. Berstad, Application of hydrogen influenced cohesive laws in the prediction of hydrogen induced stress cracking in 25%cr duplex stainless steel, *Engineering Fracture Mechanics* 75 (2008) 2333–2351.
- [8] H. Yu, J. S. Olsen, A. Alvaro, V. Olden, J. He, Z. Zhang, A uniform hydrogen degradation law for high strength steels, *Engineering Fracture Mechanics* 157 (2016) 56–71.
- [9] A. Alvaro, V. Olden, O. M. Akselsen, 3d cohesive modelling of hydrogen embrittlement in the heat affected zone of an x70 pipeline steel, *International Journal of Hydrogen Energy* 38 (2013) 7539–7549.
- [10] S. Pallaspuuro, H. Yu, A. Kisko, D. Porter, Z. Zhang, Fracture toughness of hydrogen charged as-quenched ultra-high-strength steels at low temperatures, *Materials Science and Engineering: A* 688 (2017) 190–201.
- [11] E. Martnez-Paeda, A. Golahmar, C. F. Niordson, A phase field formulation for hydrogen assisted cracking, *Computer Methods in Applied Mechanics and Engineering* 342 (2018) 742–761.
- [12] D. C. Ahn, P. Sofronis, R. H. Dodds Jr, On hydrogen-induced plastic flow localization during void growth and coalescence, *International Journal of Hydrogen Energy* 32 (2007) 3734–3742.
- [13] H. Yu, J. S. Olsen, J. He, Z. Zhang, Hydrogen-microvoid interactions at continuum scale, *International Journal of Hydrogen Energy* (2018).
- [14] H. Yu, A. C. F. Cocks, E. Tarleton, Discrete dislocation plasticity helps

- understand hydrogen effects in bcc materials, *Journal of the Mechanics and Physics of Solids* (2018).
- [15] Y. Gu, J. A. El-Awady, Quantifying the effect of hydrogen on dislocation dynamics: A three-dimensional discrete dislocation dynamics framework, *Journal of the Mechanics and Physics of Solids* (2018).
- [16] I. H. Katzarov, D. L. Pashov, A. T. Paxton, Hydrogen embrittlement i. analysis of hydrogen-enhanced localized plasticity: Effect of hydrogen on the velocity of screw dislocations in α -fe, *Physical Review Materials* 1 (2017) 033602. PRMATERIALS.
- [17] P. Sofronis, Y. Liang, N. Aravas, Hydrogen induced shear localization of the plastic flow in metals and alloys, *European Journal of Mechanics - A/Solids* 20 (2001) 857–872.
- [18] Y. Liang, D. C. Ahn, P. Sofronis, R. H. Dodds Jr, D. Bammann, Effect of hydrogen trapping on void growth and coalescence in metals and alloys, *Mechanics of Materials* 40 (2008) 115–132.
- [19] J. Koplik, A. Needleman, Void growth and coalescence in porous plastic solids, *International Journal of Solids and Structures* 24 (1988) 835–853.
- [20] C. Huang, X. Gao, T. Luo, S. M. Graham, Modeling the effect of hydrogen on ductile fracture, *Materials Performance and Characterization* 7 (2018).
- [21] A. L. Gurson, Continuum theory of ductile rupture by void nucleation and growth: Part i yield criteria and flow rules for porous ductile me-

- dia, *Journal of Engineering Materials and Technology* 99 (1977) 2–15.
10.1115/1.3443401.
- [22] V. Tvergaard, A. Needleman, Analysis of the cup-cone fracture in a round tensile bar, *Acta Metallurgica* 32 (1984) 157–169.
- [23] Z. L. Zhang, C. Thaulow, J. degrd, A complete gurson model approach for ductile fracture, *Engineering Fracture Mechanics* 67 (2000) 155–168.
- [24] Z. L. Zhang, E. Niemi, A new failure criterion for the gurson-tvergaard dilational constitutive model, *International Journal of Fracture* 70 (1994) 321–334.
- [25] T. Pardoen, J. W. Hutchinson, An extended model for void growth and coalescence, *Journal of the Mechanics and Physics of Solids* 48 (2000) 2467–2512.
- [26] K. Nahshon, J. W. Hutchinson, Modification of the gurson model for shear failure, *European Journal of Mechanics - A/Solids* 27 (2008) 1–17.
- [27] Y. Bao, T. Wierzbicki, On fracture locus in the equivalent strain and stress triaxiality space, *International Journal of Mechanical Sciences* 46 (2004) 81–98.
- [28] I. Barsoum, J. Faleskog, Rupture mechanisms in combined tension and shearmicromechanics, *International Journal of Solids and Structures* 44 (2007) 5481–5498.
- [29] V. Tvergaard, Shear deformation of voids with contact modelled by

- internal pressure, *International Journal of Mechanical Sciences* 50 (2008) 1459–1465.
- [30] M. Dunand, D. Mohr, On the predictive capabilities of the shear modified gurson and the modified mohrcoulomb fracture models over a wide range of stress triaxialities and lode angles, *Journal of the Mechanics and Physics of Solids* 59 (2011) 1374–1394.
- [31] L. Xue, Constitutive modeling of void shearing effect in ductile fracture of porous materials, *Engineering Fracture Mechanics* 75 (2008) 3343–3366.
- [32] L. E. Dhli, D. Morin, T. Brvik, O. S. Hopperstad, A lode-dependent gurson model motivated by unit cell analyses, *Engineering Fracture Mechanics* 190 (2018) 299–318.
- [33] A. U. Manual, Version 6.13-2, Dassault Systmes Simulia Corp., Providence, Rhode Island, USA (2013).
- [34] R. A. Oriani, The diffusion and trapping of hydrogen in steel, *Acta Metallurgica* 18 (1970) 147–157.
- [35] H. Yu, J. S. Olsen, J. He, Z. Zhang, Effects of loading path on the fracture loci in a 3D space, *Engineering Fracture Mechanics* 151 (2016) 22–36.
- [36] A. Gurson, Plastic flow and fracture behavior of ductile materials incorporating void nucleation, growth and coalescence, PhD Diss, Brown University (1975).

- [37] W. Jiang, Y. Li, J. Su, Modified gtn model for a broad range of stress states and application to ductile fracture, *European Journal of Mechanics - A/Solids* 57 (2016) 132–148.
- [38] Z. L. Zhang, Explicit consistent tangent moduli with a return mapping algorithm for pressure-dependent elastoplasticity models, *Computer Methods in Applied Mechanics and Engineering* 121 (1995) 29–44.
- [39] Z. L. Zhang, On the accuracies of numerical integration algorithms for gurson-based pressure-dependent elastoplastic constitutive models, *Computer Methods in Applied Mechanics and Engineering* 121 (1995) 15–28.
- [40] Z. L. Zhang, E. Niemi, A class of generalized mid-point algorithms for the gursontvergaard material model, *International Journal for Numerical Methods in Engineering* 38 (1995) 2033–2053.
- [41] R. Kiran, K. Khandelwal, Gurson model parameters for ductile fracture simulation in astm a992 steels, *Fatigue & Fracture of Engineering Materials & Structures* 37 (2014) 171–183.

1. A micromechanism based hydrogen informed Gurson model is proposed.
2. This is the first practical hydrogen embrittlement simulation tool based on HELP mechanism.
3. The model gives accurate prediction, and its calibration is straightforward and cost efficient.

Hydrogen informed Gurson model for hydrogen embrittlement simulation

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Abstract

Hydrogen-microvoid interactions were studied via unit cell analyses with different hydrogen concentrations. The absolute failure strain decreases with hydrogen concentration, but the failure loci were found to follow the same trend dependent only on stress triaxiality, in other words, the effects of geometric constraint and hydrogen on failure are decoupled. Guided by the decoupling principle, a hydrogen informed Gurson model is proposed. This model is the first practical hydrogen embrittlement simulation tool based on the hydrogen enhanced localized plasticity (HELP) mechanism. It introduces only one additional hydrogen related parameter into the Gurson model and is able to capture hydrogen enhanced internal necking failure of microvoids with accuracy; its parameter calibration procedure is straightforward and cost efficient for engineering purpose.

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Keywords: Hydrogen enhanced localized plasticity, hydrogen-microvoid interaction, Gurson model, void growth

Nomenclature

\dot{f}	Void growth rate	c	Hydrogen concentration
η	Stress triaxiality	c_L	Lattice hydrogen concentration
\bar{V}_h	Partial molar volume of hydrogen	c_T	Trapped hydrogen concentration
σ_0	Initial yield stress without hydrogen	D_L	Hydrogen diffusion coefficient
σ_e	Equivalent stress	E	Young's modulus
σ_h	Hydrostatic stress	E_b	Trap binding energy
ε_0	Strain at yielding	f_0	Initial void volume fraction
ε_e	Effective strain	f_c	Critical void volume fraction
ε_f	Failure strain	R	Universal gas constant
ε_p	Plastic strain	T	Absolute temperature

1. Introduction

Continuum level hydrogen embrittlement (HE) simulation is one of the key aspects of failure assessment and control of engineering components exposed to hydrogen environment. A sound framework for this purpose consists of three basic ingredients, namely a plausible underlying HE mechanism, a

way to determine model inputs from experiments or lower scale simulations and eventually a continuum model applicable to various geometries and loading conditions. The underlying mechanism provides the physical foundation, the input calibration method serves as a bridge linking lower scale physics (often posed in a discrete manner) and continuum mechanics, and the model as the main carrier needs to be selected depending on the other two elements.

To date, there are two prevailing HE mechanisms, hydrogen enhanced decohesion (HEDE) and hydrogen enhanced localized plasticity (HELP). The HEDE mechanism assumes that dissolved hydrogen reduces the cohesive strength of the material lattice [1]; the HELP mechanism assumes that hydrogen facilitates dislocation activity thereby enhancing plasticity locally [2]. It is straightforward to see that HEDE is compatible with Griffith type fracture, so it is favorable for the simulation of HE which is usually accompanied by brittle-like fractography [3]. In fact, HEDE based continuum level HE simulation has been in progress for over a decade, thanks to cohesive zone modeling (CZM) which well represents the brittle fracture process [4]. By lowering the cohesive strength (fracture energy) of the cohesive interface with hydrogen content, hydrogen induced premature fracture in a brittle manner can be simulated. The determination of CZM parameters in the absence of hydrogen is out of the scope and not elaborated here. Hydrogen related inputs, i.e. hydrogen effects on CZM parameters, can be obtained based on atomistic calculations or experiments. Jiang and Carter [5] performed first principles calculations and found that the ideal fracture energy decreases almost linearly with increasing hydrogen coverage. This relation was then adopted by Serebrinsky et al. [6] and Olden et al. [7] in their hy-

drogen informed CZM (HCZM) simulations. Recently, Yu et al. [8] proposed a method to calibrate hydrogen dependent cohesive laws from tension tests. The HCZM approach is now rather mature and applied widely to engineering failure assessment [9, 10]. Following a similar pattern, the phase field approach was recently applied in HE simulation [11]. In spite of its popularity, HCZM has intrinsic deficiencies. While it “physically” represents the brittle failure caused by hydrogen, it cannot represent the ductile damage in the absence of hydrogen. Due to this inconsistency, it has to be admitted in the first place that HCZM is a phenomenological approach.

In contrast to the great popularity of the HELP mechanism, HELP based continuum model for hydrogen failure prediction is yet to be developed. There could be several reasons. First, the HELP mechanism claims more plasticity in the presence of hydrogen, so one may expect ductile fracture all the time, which doesn’t agree with the brittle-like HE fractography. Therefore, one could intuitively prefer HEDE to HELP as the underlying mechanism for continuum HE modeling. Secondly, unlike the HEDE case where the DFT results of hydrogen dependent cohesive law can be readily applied to the continuum level, the HELP mechanism, while verified by theoretical calculation using a pair of dislocations [2], cannot be quantitatively applied to the continuum level, since plasticity is the collective behavior of a large dislocation aggregate on which the hydrogen effect is still unclear. Finally, even if a phenomenological form for the HELP mechanism is temporarily assumed and implemented in unit cell analyses [12], the results are only qualitative ones due to the lack of a proper failure criterion. In short, a HELP based continuum model is still lacking because the underlying theory

seems inconsistent with reality and a bridge linking different scales is lacking.

The conditions for the development of HELP based continuum model has been largely improved recently. Yu et al. [13] proposed a failure criterion associated with hydrogen induced shear band forming in unit cell analysis, which allows failure to be detected at a very small void volume fraction at low stress triaxiality regime. That is, hydrogen induced premature failure with brittle-like fractography was predicted under the HELP mechanism solely. That work also demonstrated that more plasticity does not necessarily lead to higher ductility, it therefore removed the first obstacle for adopting HELP in a continuum model. Further, a hydrogen failure locus covering a wide range of stress triaxiality was established in that work, providing inputs for the continuum model. Meanwhile, it should be noted that the link between continuum scale and lower scales is still weak, since the HELP mechanism is implemented only conceptually using a phenomenological form in the cell analyses performed so far. Most recently, a hydrogen informed three dimensional discrete dislocation dynamics (HDDD) modeling framework was established [14], incorporating the elastic stress contribution from hydrogen as Eshelby inclusion [15] and hydrogen effects on dislocation mobility calibrated based on first principles calculations [16]. Global flow behavior was simulated with this method using a microcantilever geometry and hydrogen induced global softening, consistent with the HELP mechanism, was quantitatively captured at realistic bulk hydrogen concentrations. This framework addresses hydrogen influenced large dislocation aggregate property (plasticity) at microscopic scale and can therefore serve as an ideal bridge between the atomistic and continuum scales.

With the theoretical foundation and inter-scale bridge established, the construction of HELP based continuum model is now on the agenda. Although such model is still unavailable, lots of work on the mechanics of hydrogen induced failure due to HELP has been done, providing mechanistic insights. Sofronis et al. [17] introduced HELP to mechanical analyses by implementing a hydrogen softening law which prescribes the material yield stress as a decreasing function of hydrogen concentration. This method was then adopted by Ahn et al. [12], Liang et al. [18] and implemented in unit cell analyses. By zooming into a material point represented by a void containing representative material volume, the unit cell approach is an ideal tool to investigate material failure characterized by microvoid growth and coalescence process [19]. With hydrogen softening the matrix flow stress, material failure by void coalescence along the inter-ligament was found to occur earlier, i.e. hydrogen promoted internal necking failure. In [13], a hydrogen induced shearing failure mode was identified and quantified. This failure mode is observed in low stress traxiality regime and occurs with a much smaller void size compared to that in the internal necking mode, therefore, it captures the “embrittlement” feature of hydrogen caused failure. Most recently, Huang et al. [20] studied the effect of hydrogen under different Lode parameters with unit cell approach. These studies reveal the micromechanics of hydrogen caused premature failure under the HELP theory, with a merit that the basic failure process is consistently based on microvoid activity with or without hydrogen. Therefore, they open the door to a consistently micromechanics based continuum model which could be an alternative to the phenomenological HCZM framework for continuum HE modeling.

Given the background above, the Gurson model [21] seems to be an ideal starting point for a HELP based continuum model for HE simulation. This model describes the “average” flow behavior of a single void containing representative material volume (unit cell) during the development of the void (growth and coalescence), by ”smearing“the void throughout the unit cell and then viewing the smeared cell as a material point. Regarding void coalescence as the failure event, the Gurson model is able to predict failure if a critical void volume fraction is accordingly prescribed [22]. An alternative way to predict failure is to incorporate a physically based void coalescence criterion [23, 24, 25] to the Gurson model. During the past decades, a lot of improvement and adaption have been made on this model, breeding many different versions. In general, we refer to all the versions in this family as the Gurson model. Specifically, we based our discussion on the version developed by Tvergaard and Needleman [22] in this work. The Gurson model elegantly applies the mechanics happening locally in a unit cell to global specimen level and has achieved great success in engineering practice. It is also an ideal starting point for developing new microvoid mechanism based models, for which the modification of the Gurson model for shear [26] is a typical example. About one decade ago, it was realized that the ductile failure locus is dependent not only on stress triaxiality but also on the Lode parameter [27], and this was then studied extensively using unit cell approach [28, 29]. Inspired by the micromechanics revealed in cell analyses, Nahshon and Hutchinson [26] introduced a Lode parameter dependent term to the void growth rate term, making material failure shear sensitive. Essentially, this new model regards void volume fraction as a continuum damage parameter

which is made additionally dependent on Lode parameter. Therefore, this model is not as well physically based as the original Gurson model, nevertheless, it is still micromechanism inspired and is widely adopted in practice [30]. Similar treatment on the Gurson model is found in [31] and [32].

The present work discusses the possibility of using the Gurson model to convey hydrogen-microvoid interaction mechanisms to the continuum scale. Should this work, a micromechanics inspired HELP based continuum modeling tool for HE can be delivered. This potential model is referred to as the hydrogen informed Gurson (HGurson) model hereinafter. Starting from hydrogen-microvoid interactions, a possible form of HGurson model is proposed, together with a suitable parameter calibration procedure. At the moment, we don't aim to deliver a complete HGurson model ready for use, given the complexity in hydrogen assisted microvoid failure process. Instead, we elaborate the challenges in the development of such a model, propose solutions for some of them and leave the rest for future study. As a brief overview, the challenges/complexities include (but are not limited to): hydrogen trapping, change of failure mode in different stress triaxiality regime, inhomogenous material softening due to hydrogen redistribution and the form of hydrogen softening law. Being aware of all these complexities, we hereby limit our focus to a simple case with a linear softening law in high triaxiality regime, and a prototype HGurson model is presented.

2. Hydrogen-microvoid interactions

Hydrogen microvoid interactions are investigated via hydrogen diffusion coupled unit cell analyses [13]. J2 flow theory with isotropic hardening is

applied to describe the plastic flow in the matrix material

$$\sigma_f = \sigma_0(c) \left(1 + \frac{\varepsilon_p}{\varepsilon_0}\right)^n \quad (1)$$

where σ_f is the flow stress, $\sigma_0(c)$ the initial yield stress which is a function of the total hydrogen concentration c , ε_p the plastic strain and $\varepsilon_0 = \sigma_0/E$ the corresponding yield strain with E being the Young's modulus. To account for the HELP mechanism, the flow stress in the matrix material is assumed to decrease with hydrogen content. More specifically, the initial yield stress σ_0 is prescribed as a decreasing function of hydrogen concentration, for which the linear form [12] is most widely adopted

$$\sigma_0(c) = \begin{cases} [(\xi - 1)\frac{c}{c_L^0} + 1]\sigma_0 & \sigma_0(c) > \zeta\sigma_0 \\ \zeta\sigma_0 & \sigma_0(c) \leq \zeta\sigma_0 \end{cases} \quad (2)$$

where σ_0 is the initial yield stress with zero hydrogen concentration, $\xi\sigma_0$ the initial yield stress at the initial lattice hydrogen concentration c_L^0 and $\zeta\sigma_0$ the lowest possible value of the yield stress considering that hydrogen cannot cause the yield stress to vanish in reality.

The total hydrogen population consists of the lattice hydrogen residing at normal interstitial lattice sites and the trapped hydrogen residing at dislocation traps

$$c = c_L + c_T \quad (3)$$

where c_L is the lattice hydrogen concentration and c_T the trapped hydrogen

concentration. These two quantities can be further expressed as

$$c_L = \theta_L N_L \quad c_T = \theta_T N_T \quad (4)$$

where θ_L is the fraction of occupied interstitial lattice sites and N_L the lattice site density; similarly, θ_T is the fraction of occupied trapping sites and N_T the trapping site density.

Assuming steady state hydrogen distribution, the material flow stress is dependent on the hydrostatic stress field and the plastic strain field, which can be implemented to realize hydrogen coupled unit cell analysis [12]. Alternatively, transient hydrogen diffusion analysis can be directly coupled with unit cell analysis [13], which can be realized with the help of user subroutines in a commercial finite element software such as ABAQUS [33]. Under the limit of sufficient diffusion time, these approaches are equivalent, and the latter is adopted in this work. Transient hydrogen diffusion is governed by

$$\frac{\partial c_L}{\partial t} + \frac{\partial c_T}{\partial t} - \nabla \cdot (D_L \nabla c_L) + \nabla \cdot \left(\frac{D_L c_L \bar{V}_h}{RT} \nabla \sigma_h \right) = 0 \quad (5)$$

where D_L stands for the lattice diffusivity coefficient, \bar{V}_h the partial molar volume of hydrogen and σ_h the hydrostatic stress. An equilibrium exists between hydrogen in lattice sites and in trapping sites [34]

$$\frac{\theta_T}{1 - \theta_T} = \frac{\theta_L}{1 - \theta_L} K_T \quad (6)$$

where K_T is the trap equilibrium constant $K_T = \exp(-E_b/RT)$ with E_b being the trap binding energy, R the universal gas constant and T the absolute

temperature.

The unit cell method focuses on a single void behavior in a representative material volume with periodic boundary condition. It offers accurate control over loading path and is an ideal approach to construct material failure loci [35]. The failure locus is defined as a relation between the effective strain at failure ε_f and the geometric constraint. The level of geometric constraint can be characterized by stress triaxiality and Lode parameter [13]. In this work, the cylindrical unit cell [19] under proportional loading is employed, leading to an axisymmetric loading scenario where the Lode parameter remains constant $L \equiv -1.0$. In other words, 2D failure loci are concerned throughout this work. The effective strain of the unit cell is defined as [19]

$$\varepsilon_e = \frac{2}{3}|\varepsilon_3 - \varepsilon_1|, \quad (7)$$

where $\varepsilon_3 = \ln(L/L_0)$ and $\varepsilon_1 = \ln(R/R_0)$, with L and R being the current cell height and radius, respectively. And the level of constraint is characterized by stress triaxiality

$$\eta = \frac{\sigma_h}{\sigma_e}, \quad (8)$$

with σ_e being the equivalent stress.

With a similar approach, we studied the effect of hydrogen on material failure loci in a previous work [13] and a complicated picture was revealed. The effect was found to depend on hydrogen trap strength as well as stress triaxiality. With weak trapping, failure occurred in internal necking mode over the entire range of triaxiality, and hydrogen promoted this failure mode. With strong trapping, hydrogen induced the formation of a shear band in

the low triaxiality regime, giving rise to a new internal shearing failure mode. This adds complexity to the development of the HGurson model. Ultimately, a successful HGurson model is expected to reproduce the hydrogen failure loci, capturing all the complexities involving trapping strength dependency and different failure modes. This work as a starting point, is devoted only to capturing hydrogen promoted internal necking failure mode, which is the first issue that should be addressed in model development. In other words, we limit our focus here to the medium and high stress triaxiality regime $\eta > 1.0$.

Hydrogen diffusion coupled unit cell analysis describes the mechanical process in a representative material volume, which is viewed as a material point at the specimen level. Therefore, HGurson model is essentially a homogenized description of hydrogen-microvoid interactions at material points. In this sense, the cell analyses can be regarded as “virtual experiments” that can be used as reference to calibrate and validate the HGurson model. Such “virtual experiments” need to be performed with various hydrogen concentrations. In all the cell analyses here, the Young’s modulus is $E = 2 \times 10^5 \text{MPa}$, the initial yield stress of the material is $\sigma_0 = 400 \text{MPa}$, and the strain hardening exponent is $n = 0.1$. The initial void volume fraction of the unit cell is $f_0 = 0.0013$ in all simulations. The linear hydrogen softening law in [Equation 2](#) is adopted with $\xi = 0.9$ and $\zeta = 0.5$. Lattice hydrogen properties relevant to steel are adopted: the lattice site density is taken as $N_L = 8.74 \times 10^{19}$ sites/ mm^3 , the partial molar volume of hydrogen as $\bar{V}_h = 2 \times 10^3 \text{mm}^3/\text{mol}$ and lattice diffusion coefficient as $D_L = 2.5 \times 10^{-11} \text{m}^2/\text{s}$. The same trapping parameters as in [\[13\]](#) representing a strong trapping scenario are adopted. The reference hydrogen concentration ([Equation 2](#)) at which a 10% reduc-

tion in yield stress is observed is assumed to be $c_L^0 = 1.0\text{wppm}$. The loading rate during simulation is sufficiently low so that steady state hydrogen distribution is guaranteed. It should be noted that the assumed level of hydrogen softening is very large. This is for a larger contrast between hydrogen and original failure loci and for a better demonstration of the decoupling principle. With less softening, the principle and the HGurson model still apply well, except that the absolute difference in the failure loci is less pronounced. To give a sense of how the magnitude of the effect of hydrogen depends on the softening parameters, we include unit cell results with milder hydrogen softening, a 5% reduction and a 1% reduction with $c_L^0 = 1.0\text{wppm}$, in [Appendix A](#).

Four cases with different initial uniform hydrogen concentrations $c_0 = 0.5, 1.0, 1.5, 2.0\text{wppm}$ and a hydrogen free case $c_0 = 0$ are investigated. Unit cell analyses are performed under fixed stress triaxiality ranging from $\eta = 1.0$ to $\eta = 3.0$ with an interval of 0.2. Over this range, only hydrogen promoted internal necking failure is observed. The failure loci are constructed for each hydrogen concentration.

The results of hydrogen coupled unit cell analyses, quantified as failure loci, are presented in [Fig. 1](#). Internal necking failure is observed over the entire range of triaxiality in all cases, and the failure strain decreases with the increase of hydrogen concentration.

Before establishing a model to capture these failure loci, the mechanism of hydrogen promoted internal necking failure needs to be analyzed. An intuitive impression is that hydrogen induced softening of the matrix material accounts for the early failure, since the initial yielding stress lowers

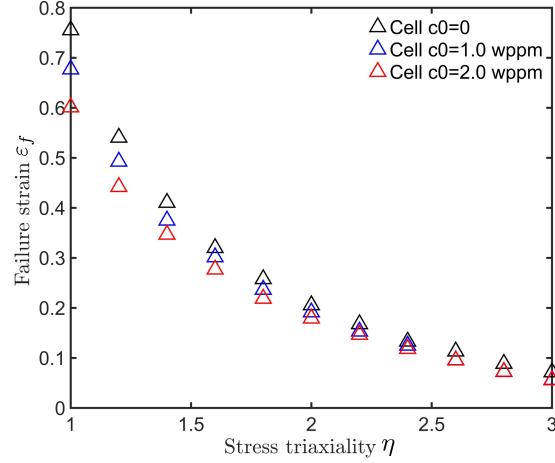


Fig. 1 The failure loci obtained by hydrogen diffusion coupled unit cell analyses, with and without hydrogen.

as c_0 increases. Looking into the hydrogen distribution contour during the loading process, another possible reason is spotted. Due to the pressure and plastic strain dependent nature of hydrogen redistribution, higher hydrogen concentration is built up at the inter-ligament region, which in turn leads to non-uniform hydrogen softening across the unit cell, as shown in Fig. 2. This could also be a rationale for the premature failure. To distinguish between these causes, we refer to the former rationale as hydrogen caused uniform softening and the latter as hydrogen caused non-uniform softening.

To probe the actual cause, an artificial case where the initial yield stress of the matrix material is decreased uniformly by 50% (the lower bound of hydrogen softening) was simulated. The void growth curves in this case and in the realistic cases with and without hydrogen are plotted in Fig. 3. Clearly, hydrogen caused uniform softening in the matrix material contributes little to the acceleration in void growth and premature failure, indicating hydrogen

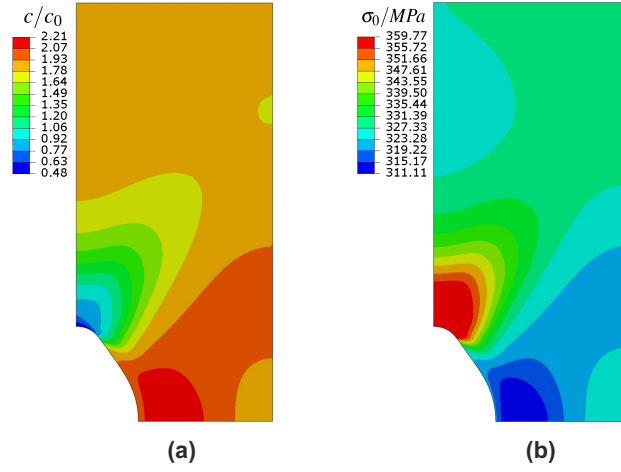


Fig. 2 (a) The distribution of hydrogen concentration and (b) the initial yield stress contours at an effective strain $\epsilon_e = 0.5$ and stress triaxiality $\eta = 1.0$, obtained with hydrogen $c_0 = 1.0$ wppm.

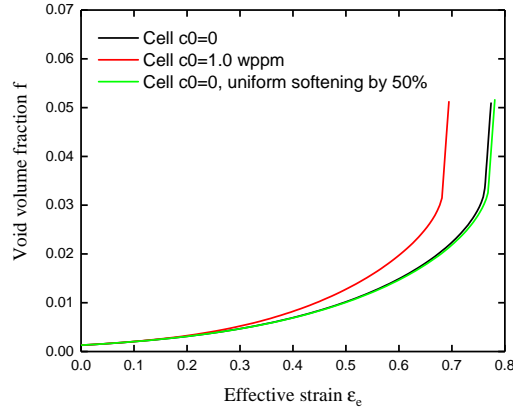


Fig. 3 Void growth curves obtained via unit cell analyses at stress triaxiality $\eta = 1.0$, including the hydrogen free case, a hydrogen case and an artificial case where no hydrogen is present but the entire matrix material is uniformly softened by 50%.

caused non-uniform softening plays a dominant role. This provides important reference for subsequent model development.

3. HGurson formulation

Coming back to the failure loci in Fig. 1, it is observed that they generally follow a same trend, which is clearly demonstrated by applying a normalization scheme as shown in Fig. 4(a). The scheme was performed by normalizing

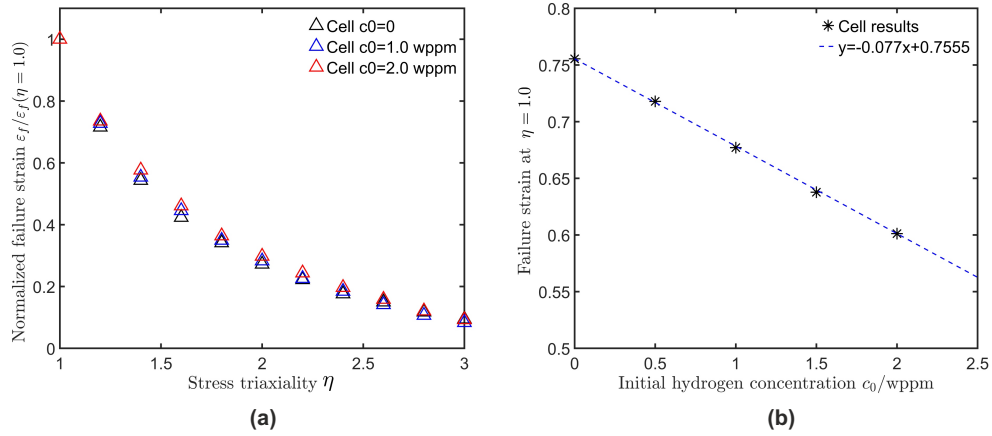


Fig. 4 (a) The normalized failure loci; the failure loci approximately collapse into one curve upon normalization. (b) The value used for normalization versus initial hydrogen concentration, which shows a linear relation.

the failure strain values on each failure locus by the value corresponding to $\eta = 1.0$ on the same locus. After normalization, all the failure loci, including the hydrogen free failure locus, collapsed into one curve, verifying that they have the same triaxiality dependence, so the presence of hydrogen just scales the absolute value of a specific locus. In other words, it indicates the failure strain $\varepsilon_f(\eta, c)$ which is a function of stress triaxiality and hydrogen concentration can be expressed in a decoupled form

$$\varepsilon_f(\eta, c) = f(\eta) \cdot h(c) \quad (9)$$

with $f(\eta)$ determined in Fig. 4(a) and $h(c)$ in Fig. 4(b). It should be noted that $h(c)$ is a “hydrogen scaling” function that is calibrated from the “virtual experiments” instead of a fitting parameter. The decoupling phenomenon has been observed in the case without trapping as well as in the current case. It may be attributed to the fact that the same failure mechanism, i.e. hydrogen induced local softening and the similar softening pattern, e.g. Fig. 2(b), apply at different hydrogen concentrations. This decoupling principle holds true as long as the hydrogen induced local softening occurs at the inter-ligament, which is the case in the high triaxiality regime concerned here. In the low triaxiality regime where internal shearing failure is observed [13], this principle needs to be verified separately. The fact that the hydrogen free case also follows this rule suggests that we can start from a hydrogen free mechanical model and then incorporate the scaling due to hydrogen to capture the hydrogen failure loci. To predict failure of microvoids without hydrogen, the Gurson model is a perfect candidate.

3.1. Gurson model

The Gurson model [36] is a popular approach to describing failure in porous materials. In 1975, Gurson [36] studied the macroscopic plastic flow of a long circular cylindrical void in a matrix of rigid-plastic von Mises material. By utilizing an approximate velocity field and appropriate boundary values at the outer and void surface, an upper bound yield function was derived

$$\phi(\boldsymbol{\sigma}, \bar{\sigma}, f) = \left(\frac{\sigma_e}{\bar{\sigma}}\right)^2 + 2q_1 f \cosh\left(\frac{q_2 \sigma_m}{2\bar{\sigma}}\right) - 1 - q_3 f^2 = 0 \quad (10)$$

where $\boldsymbol{\sigma}$ is the stress tensor and f the void volume fraction; σ_e is the macroscopic equivalent stress and σ_m the mean stress. q_1 , q_2 and $q_3 = q_1^2$ are the parameters introduced by Tvergaard and Needleman [22] in order to enhance the fitting capacity. This modified version is usually referred to as the GTN model [37], and the original Gurson model is retrieved by setting q_1 , q_2 and q_3 to 1. In this model, the porous material is represented by a void free continuum, and the microvoids are “smeared” across the continuum.

When loaded, the void volume fraction f of the material increases due to microvoid growth, and the yield surface is modified following Equation 10. The rate of void volume change \dot{f} , i.e. void growth rate is derived from the mass conservation condition in the matrix

$$\dot{f} = (1 - f)D_{kk}^P \quad (11)$$

where D_{kk}^P is the volumetric strain rate. It is assumed that failure initiates when the void volume fraction reaches a critical value $f = f_c$. Therefore, f could be regarded as a damage parameter with a sound micromechanical basis.

The GTN version is employed here to capture the microvoid failure locus in the absence of hydrogen. Consistent with the unit cell analyses, the material initially possesses a void volume fraction $f_0 = 0.0013$ and void nucleation is not taken into account. The same mechanical properties for the unit cell matrix are assigned to the Gurson matrix. Unit cell analyses show that the critical void volume fraction at failure initiation is around 0.03, therefore, $f_c = 0.03$ is adopted in the Gurson model. A single element model assigned with Gurson material is employed, in order to verify the predictions against

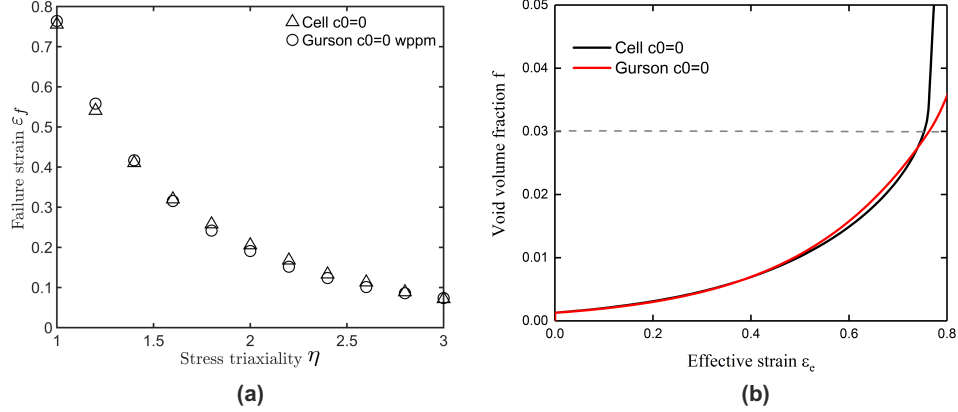


Fig. 5 Using the Gurson model to capture (a) hydrogen free failure locus and (b) void growth in the case with stress triaxiality $\eta = 1.0$.

the cell results. This element corresponds to the material point represented by the unit cell in [section 2](#). The same loading conditions, e.g. fixed stress triaxiality, are applied to the single element model as to the unit cell. The GTN fitting parameters are selected as $q_1 = 1.3$, $q_2 = 1.0$, $q_3 = 1.69$, which yields the best prediction of the hydrogen free failure locus. The Gurson model predictions of unit cell failure locus and void growth in the case of $\eta = 1.0$ are presented in [Fig. 5](#). Good agreement between the model prediction and the cell results are achieved.

3.2. HGurson model

Following the decoupling principle revealed in the previous section, we now proceed to incorporate the effect of hydrogen into the Gurson model established above. Since the material point is represented by only one element in the HGurson model, hydrogen redistribution observed in the unit cell analyses cannot be directly captured. Therefore, the hydrogen concen-

tration that is passed to the model has to be the initial uniform hydrogen concentration applied to the unit cell: again, the entire hydrogen-microvoid interactions, including hydrogen redistribution and plasticity localization are captured in a homogenized manner by the HGurson model. Recall that it is the hydrogen caused non-uniform softening that is dominant in the premature failure, but this cannot be reflected directly in the single element model. Looking at the derivation of the original Gurson model, we face the same dilemma: the Gurson model was derived assuming an isotropic matrix with uniform mechanical property, therefore, hydrogen can only soften the entire volume, in other words, there is no way to implement non-uniform hydrogen softening, if we wish to rigorously keep the original formulation of the Gurson model.

To demonstrate the deficiency of considering only the hydrogen caused uniform softening effect in HGurson model, we use a simple artificial case where the single element Gurson model is simulated at $\eta = 1.0$ and the initial yield stress of the matrix material is decreased by 50% uniformly. This artificial HGurson case corresponds to the artificial cell case in [Fig. 3](#). The void growth curve has been included in [Fig. 8\(a\)](#). Clearly, directly implementing uniform softening to the Gurson model has little influence on void growth and therefore does not help capture the hydrogen failure loci.

To account for the hydrogen caused non-uniform softening effect in the HGurson model, the rigorous way is to reformulate the original Gurson model to consider a local softening regime in the void ligament. The solution will be extremely difficult, if not impossible, and it requires quantitative description of hydrogen induced non-uniform softening when it comes to the HGurson

model, which induces further complexity. An alternative way is to view the Gurson model as a damage model and the void volume fraction f a damage parameter, so that the premature failure can be attributed to the hydrogen promoted accumulation of damage. The latter is adopted in this work, inspired by the practice in [26] which introduced the influence of external shearing to the Gurson model.

The strategy is therefore to let hydrogen accelerate damage accumulation in the Gurson model, and the acceleration should be dependent on hydrogen concentration. For this purpose, the void growth rate \dot{f} is made additionally dependent on the initial hydrogen concentration c_0 applied to the material point. It should be noted that c_0 is referred to as the initial concentration in the sense that it prescribes the hydrogen condition at the beginning of hydrogen-microvoid interaction, at each material point and for a given time step in HGurson simulation. At the specimen level, c_0 should correspond to the transient hydrogen concentration at materials points instead of the global concentration initially applied to the whole specimen. In the lack of further information on hydrogen accelerated damage accumulation, the linear scaling function stands as a natural option [26]

$$\dot{f}(c_0) = \dot{f}_0 \cdot k_H(c_0) = (1 - f)D_{kk}^P \cdot k_H(c_0) \quad (12)$$

As to be shown later, this function can yield satisfactory failure prediction. In this formulation, the void growth rate in the presence of hydrogen is simply the hydrogen free void growth rate $\dot{f}_0 = \dot{f}(c_0 = 0)$ multiplied by a scaler as a function of hydrogen concentration at the material point. In the case of the single element model, since the initial hydrogen concentration is constant,

this scaler is a constant. Therefore, this scaler function can be calibrated via comparison between the single element model and unit cell results.

Applying [Equation 12](#) and keeping all the other parameters unchanged, the void growth rate will be accelerated. However, it is not easy to evaluate the acceleration analytically, since the volumetric strain rate D_{kk}^P in this expression will also be increased due to the modification. Assuming D_{kk}^P remains constant throughout the simulation, we have

$$\int_0^{\varepsilon_{f0}} \dot{f}_0 d\varepsilon = f_c \quad (13)$$

$$k_H(c_0) \cdot \int_0^{\varepsilon_f(c_0)} \dot{f}_0 d\varepsilon = f_c \quad (14)$$

where ε_{f0} denotes the hydrogen free failure strain. [Equation 14](#) indicates the hydrogen failure strain $\varepsilon_f(c_0)$ is equivalent to the strain value corresponding to the void volume fraction $f_c/k_H(c_0)$ in the hydrogen free case. In the simplest scenario where \dot{f}_0 is constant, i.e. the void growth curve is linear, we have

$$k_H(c_0) = \frac{\varepsilon_{f0}}{\varepsilon_f(c_0)} \quad (15)$$

In practice, however, the void growth curve is concave up as shown in [Fig. 6](#). In this figure, the actual failure strains are $\varepsilon_f = 0.682$ and $\varepsilon_f = 0.764$ in the $c_0 = 1.0wppm$ and $c_0 = 0$ cases, respectively. Due to the linear void growth assumption, the scaler is determined as $k_H = 1.16$, yielding a prediction of $\varepsilon_f = 0.733$, $\approx 7.5\%$ higher than the actual value. Therefore, the linear void growth assumption leads to overestimation. Meanwhile, it is noted that the

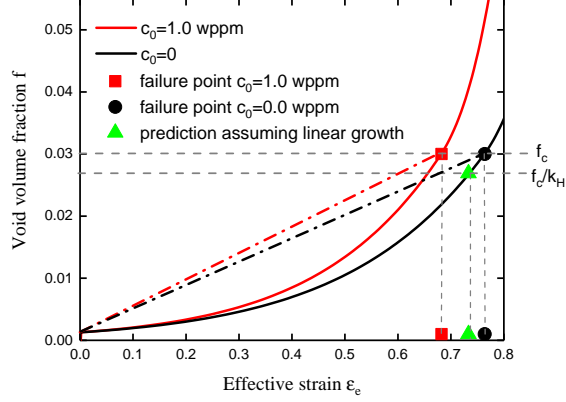


Fig. 6 The prediction of hydrogen failure point using Equation 14 and assuming linear void growth. The solid lines represent the actual void growth curves extracted from HGurson simulations, and the dashed dotted lines represent the assumed linear void growth line. k_H is determined as $k_H = \frac{\varepsilon_{f0}}{\varepsilon_f(c_0=1.0wppm)}$.

discussion above is based on the assumption that D_{kk}^P remains constant after implementing Equation 12. As a matter of fact, D_{kk}^P is found to increase in the simulation with hydrogen, scaled up approximately by a factor of $\alpha \cdot \varepsilon_e$, with $\alpha > 1.0$ roughly being a constant and ε_e the effective strain. This implies the failure strain predicted with Equation 14 and Equation 15 in practice will be smaller than that estimated in Fig. 6. In other words, the overestimation eventually will be less than 7.5%, making the prediction rather satisfactory.

Going back to Fig. 4 and Equation 9, we now have

$$k_H(c_0) = \frac{\varepsilon_f(\eta, 0)}{\varepsilon_f(\eta, c_0)} = \frac{h(0)}{h(c_0)}, \quad (16)$$

so the parameter k_H is a function of c_0 and independent of stress triaxiality.

k_H as a function of c_0 can then be calibrated based on Fig. 4(b)

$$k_H(c_0) = 0.16c_0 + 1.0. \quad (17)$$

It should be emphasized that this function is obtained via calibration of the unit cell failure loci following the decoupling principle, rather than out of pure fitting.

The HGurson model is established by implementing Equation 12 and Equation 17. This model is then implemented via user defined material subroutine UMAT in ABAQUS [33], using the explicit consistent tangent modulus method [38, 39, 40]. The hydrogen failure loci predicted by the single element HGurson model for the cases $c_0 = 1.0wppm$ and $c_0 = 2.0wppm$ are shown in Fig. 7. Satisfactory agreement between the HGurson predictions

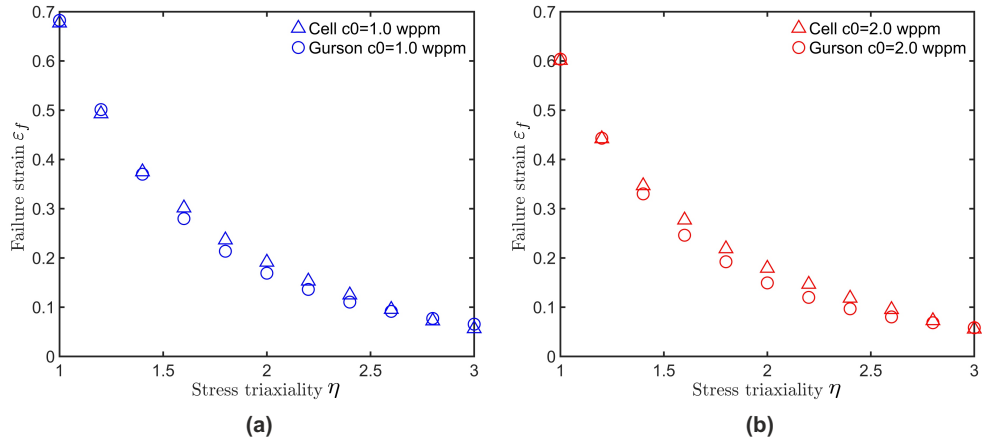


Fig. 7 Single element HGurson model prediction of hydrogen failure loci for (a) $c_0 = 1.0wppm$ and (b) $c_0 = 2.0wppm$.

and the unit cell results is achieved. Except for the failure strain, the void growth curve and stress-strain relation are also captured with good accuracy,

which is verified by comparing the HGurson and unit cell results with $\eta = 1.0$ and $c_0 = 1.0\text{wppm}$, as shown in Fig. 8.

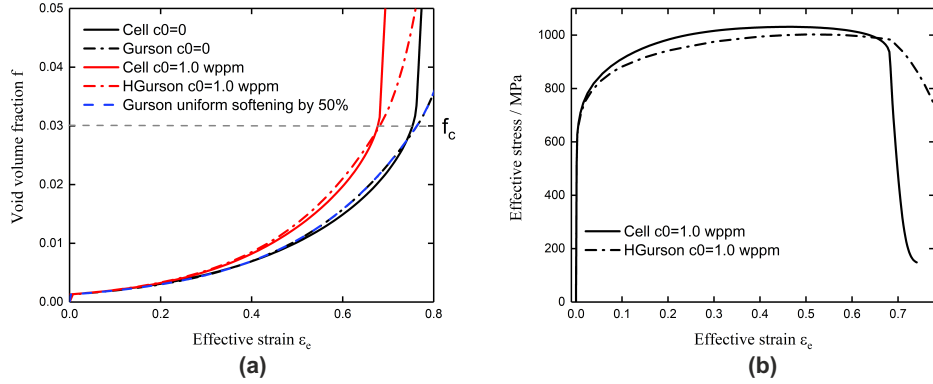


Fig. 8 The HGurson model prediction of (a) void growth curve and (b) effective stress-strain relation for the case with $\eta = 1.0$ and $c_0 = 1.0\text{wppm}$. The void growth curves without hydrogen and a (artificial) void growth curve obtained by softening the original Gurson model uniformly are also included in (a).

So far, an HGurson model accounting for hydrogen enhanced internal necking failure has been delivered. This model reproduces the “virtual experimental” results obtained via hydrogen diffusion coupled unit cell analyses. For a given material, this model keeps all the hydrogen free material properties calibrated for the Gurson model and introduces only one additional hydrogen acceleration of void (damage) growth term $k_H(c_0)$, which is dependent only on hydrogen concentration c_0 . In real life, the void behaviour is more complicated, accompanied by rotation and shape change. These will inevitably affect model parameters, such as the critical void volume fraction f_c and the q parameters in the GTN version. To consider the hydrogen dependence of these parameters, more parameters and assumptions have to be included and additional calibrations are required, rendering the model redun-

dant. Following the decoupling principle regarding the effect of hydrogen, we keep all the Gurson parameters unaffected by hydrogen, once they are determined in the hydrogen free case. This yields a clean HGurson model with good accuracy. Similar practice is found in the shear modified Gurson model [26]. As noted before, c_0 is the initial uniform hydrogen concentration in the single element model, but it will be the real time hydrogen concentration at material points in specimen level simulations. The application of Equation 2 will cause softening to plastic flow, which will occur mainly at the failure process zone where a high concentration of hydrogen is built up. In most part of the specimen, hydrogen concentration will remain low and therefore the global loading curve is not expected to be severely softened.

The HGurson model is of practical value for engineering failure assessment to which material failure locus is critical. To calibrate a failure locus, the conventional way is to design test specimens with various geometries representing a range of stress triaxialities; the specimens are then loaded to failure so that the relation between failure strain and stress triaxiality can be obtained. For hydrogen failure assessment, the whole procedure has to be repeated under different hydrogen concentrations, in order to construct hydrogen failure loci as shown in Fig. 1, which increases the workload by several times. Inspired by the decoupling principle revealed in Fig. 4, the calibration procedure for the HGurson model and hence for failure loci can be significantly simplified:

- (I) A series of mechanical tests with different geometries (stress triaxialities) in the absence of hydrogen need to be performed on a given material, yielding hydrogen free Gurson model parameters (hydrogen

free failure locus), e.g. [41].

- (II) Hydrogen charged mechanical tests need to be performed using any (one) geometry at several hydrogen concentrations to produce a hydrogen degradation curve similar to that in Fig. 4(b), and the hydrogen related term $k_H(c_0)$ (Equation 17) can then be determined.

In this procedure, different geometries need to be tested only in step (I), which is the necessary cost for material calibration in the absence of hydrogen. In step (II), utilizing the decoupling concept, only one specimen geometry is needed and only a couple of hydrogen concentrations need to be tested. Therefore, this HGurson model calibration procedure is cost efficient for engineering purpose.

4. Summary

A hydrogen informed Gurson model for hydrogen enhanced internal necking failure in high stress triaxiality regime was established in this work, as the first step towards a practical hydrogen embrittlement simulation tool based on the HELP mechanism.

Using hydrogen diffusion coupled unit cell analyses as “virtual experiments”, hydrogen enhanced internal necking failure loci were constructed at various concentrations and an important conclusion in hydrogen-microvoid interactions, i.e. the decoupling principle, was drawn. The hydrogen failure strain was shown to be a decreasing function of stress triaxiality and hydrogen concentration, and more importantly, the effects of these two factors were found to be decoupled. Further investigation demonstrated that hydrogen caused non-uniform softening of the unit cell matrix is the dominant factor

in hydrogen enhanced internal necking failure. These conclusions hold for a wide range of hydrogen trapping strength, as far as internal necking failure is concerned.

The HGurson model was proposed based these findings. Inspired by the decoupling concept, this model uses the Gurson model which accurately captures the hydrogen free microvoid process as the basis and introduces only one hydrogen related term to accelerate damage accumulation. Due to the clean formulation and the easy calibration of the hydrogen related term, the proposed model is user friendly and cost efficient for engineering practice. Good agreement between the HGurson model predictions and the “virtual experimental” results were achieved.

The HGurson model derivation was demonstrated using a strong hydrogen trapping case, since it gives pronounced hydrogen degradation in failure strain. In fact, we also studied the case with no hydrogen trapping and found that the model possesses the same form and follows the same derivation procedure. Therefore, this HGurson model is expected to apply to various hydrogen trapping strengths as far as internal necking failure mode is concerned.

This work concerns only hydrogen enhanced internal necking failure and is just the first step towards a HELP mechanism based hydrogen embrittlement simulation tool. To deliver a complete model applicable to the entire range of stress triaxiality, hydrogen induced internal shearing should also be addressed, which will be our next step.

Acknowledgements

The financial support from Aker Solutions and NTNU via the Integrity of Ni-Alloys for Subsea Applications (INASA) project is greatly acknowledged. We also want to thank the Research Council of Norway for funding through the Hydrogen-induced degradation of offshore steels in ageing infrastructure - models for prevention and prediction (HIPP). Contract No. 234130/E30.

Appendix A. Failure loci under milder hydrogen softening

In order to give a sense of how the magnitude of the effect of hydrogen depends on the softening parameters, we present the failure loci obtained using $\xi = 0.95, c_L^0 = 1.0\text{wppm}$ and $\xi = 0.99, c_L^0 = 1.0\text{wppm}$ (Equation 2). With milder hydrogen softening, the decrease in failure strain due to hy-

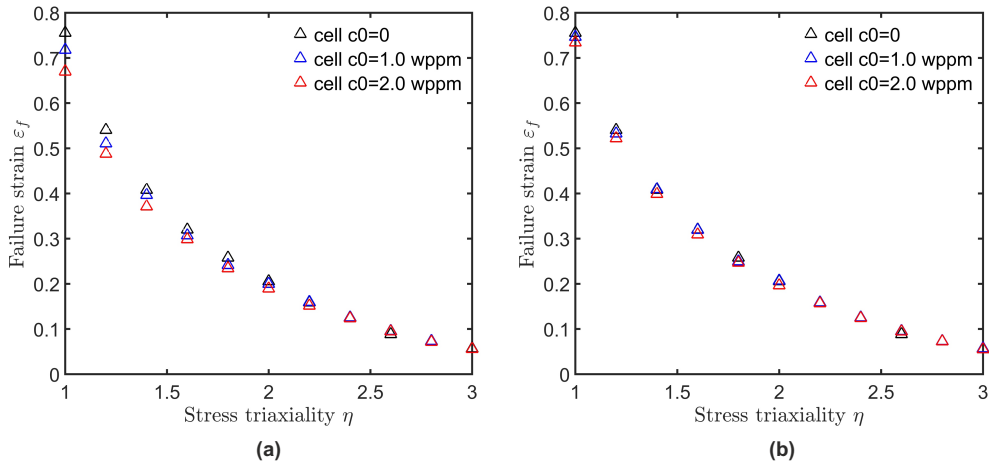


Fig. A.9 Failure loci obtained using unit cell analyses with milder hydrogen softening: (a) $\xi = 0.95, c_L^0 = 1.0\text{wppm}$ and (b) $\xi = 0.99, c_L^0 = 1.0\text{wppm}$.

drogen becomes smaller. However, the shape of failure loci are the same as that in Fig. 1; it has been verified that the decoupling principle, e.g. Fig. 4

and [Equation 9](#) still holds. Therefore, the HGurson model formulation also applies in these cases with milder hydrogen softening.

References

- [1] R. A. Oriani, A mechanistic theory of hydrogen embrittlement of steels, *Berichte der Bunsengesellschaft für physikalische Chemie* 76 (1972) 848–857.
- [2] H. K. Birnbaum, P. Sofronis, Hydrogen-enhanced localized plasticity mechanism for hydrogen-related fracture, *Materials Science and Engineering: A* 176 (1994) 191–202.
- [3] H. Yu, Modelling and assessment of hydrogen embrittlement in steels and nickel alloys, PhD Diss, Norwegian University of Science and Technology (2003).
- [4] H. Khoramishad, J. Akbardoost, M. Ayatollahi, Size effects on parameters of cohesive zone model in mode I fracture of limestone, *International Journal of Damage Mechanics* 23 (2014) 588–605.
- [5] D. E. Jiang, E. A. Carter, First principles assessment of ideal fracture energies of materials with mobile impurities: implications for hydrogen embrittlement of metals, *Corrosion Reviews* 52 (2004) 4801–4807.
- [6] S. Serebrinsky, E. A. Carter, M. Ortiz, A quantum-mechanically informed continuum model of hydrogen embrittlement, *Journal of the Mechanics and Physics of Solids* 52 (2004) 2403–2430.

- [7] V. Olden, C. Thaulow, R. Johnsen, E. stby, T. Berstad, Application of hydrogen influenced cohesive laws in the prediction of hydrogen induced stress cracking in 25%cr duplex stainless steel, *Engineering Fracture Mechanics* 75 (2008) 2333–2351.
- [8] H. Yu, J. S. Olsen, A. Alvaro, V. Olden, J. He, Z. Zhang, A uniform hydrogen degradation law for high strength steels, *Engineering Fracture Mechanics* 157 (2016) 56–71.
- [9] A. Alvaro, V. Olden, O. M. Akselsen, 3d cohesive modelling of hydrogen embrittlement in the heat affected zone of an x70 pipeline steel, *International Journal of Hydrogen Energy* 38 (2013) 7539–7549.
- [10] S. Pallaspuuro, H. Yu, A. Kisko, D. Porter, Z. Zhang, Fracture toughness of hydrogen charged as-quenched ultra-high-strength steels at low temperatures, *Materials Science and Engineering: A* 688 (2017) 190–201.
- [11] E. Martnez-Paeda, A. Golahmar, C. F. Niordson, A phase field formulation for hydrogen assisted cracking, *Computer Methods in Applied Mechanics and Engineering* 342 (2018) 742–761.
- [12] D. C. Ahn, P. Sofronis, R. H. Dodds Jr, On hydrogen-induced plastic flow localization during void growth and coalescence, *International Journal of Hydrogen Energy* 32 (2007) 3734–3742.
- [13] H. Yu, J. S. Olsen, J. He, Z. Zhang, Hydrogen-microvoid interactions at continuum scale, *International Journal of Hydrogen Energy* (2018).
- [14] H. Yu, A. C. F. Cocks, E. Tarleton, Discrete dislocation plasticity helps

- understand hydrogen effects in bcc materials, *Journal of the Mechanics and Physics of Solids* (2018).
- [15] Y. Gu, J. A. El-Awady, Quantifying the effect of hydrogen on dislocation dynamics: A three-dimensional discrete dislocation dynamics framework, *Journal of the Mechanics and Physics of Solids* (2018).
- [16] I. H. Katzarov, D. L. Pashov, A. T. Paxton, Hydrogen embrittlement i. analysis of hydrogen-enhanced localized plasticity: Effect of hydrogen on the velocity of screw dislocations in α -fe, *Physical Review Materials* 1 (2017) 033602. PRMATERIALS.
- [17] P. Sofronis, Y. Liang, N. Aravas, Hydrogen induced shear localization of the plastic flow in metals and alloys, *European Journal of Mechanics - A/Solids* 20 (2001) 857–872.
- [18] Y. Liang, D. C. Ahn, P. Sofronis, R. H. Dodds Jr, D. Bammann, Effect of hydrogen trapping on void growth and coalescence in metals and alloys, *Mechanics of Materials* 40 (2008) 115–132.
- [19] J. Koplik, A. Needleman, Void growth and coalescence in porous plastic solids, *International Journal of Solids and Structures* 24 (1988) 835–853.
- [20] C. Huang, X. Gao, T. Luo, S. M. Graham, Modeling the effect of hydrogen on ductile fracture, *Materials Performance and Characterization* 7 (2018).
- [21] A. L. Gurson, Continuum theory of ductile rupture by void nucleation and growth: Part i yield criteria and flow rules for porous ductile me-

- dia, *Journal of Engineering Materials and Technology* 99 (1977) 2–15.
10.1115/1.3443401.
- [22] V. Tvergaard, A. Needleman, Analysis of the cup-cone fracture in a round tensile bar, *Acta Metallurgica* 32 (1984) 157–169.
- [23] Z. L. Zhang, C. Thaulow, J. degrd, A complete gurson model approach for ductile fracture, *Engineering Fracture Mechanics* 67 (2000) 155–168.
- [24] Z. L. Zhang, E. Niemi, A new failure criterion for the gurson-tvergaard dilational constitutive model, *International Journal of Fracture* 70 (1994) 321–334.
- [25] T. Pardoen, J. W. Hutchinson, An extended model for void growth and coalescence, *Journal of the Mechanics and Physics of Solids* 48 (2000) 2467–2512.
- [26] K. Nahshon, J. W. Hutchinson, Modification of the gurson model for shear failure, *European Journal of Mechanics - A/Solids* 27 (2008) 1–17.
- [27] Y. Bao, T. Wierzbicki, On fracture locus in the equivalent strain and stress triaxiality space, *International Journal of Mechanical Sciences* 46 (2004) 81–98.
- [28] I. Barsoum, J. Faleskog, Rupture mechanisms in combined tension and shearmicromechanics, *International Journal of Solids and Structures* 44 (2007) 5481–5498.
- [29] V. Tvergaard, Shear deformation of voids with contact modelled by

- internal pressure, *International Journal of Mechanical Sciences* 50 (2008) 1459–1465.
- [30] M. Dunand, D. Mohr, On the predictive capabilities of the shear modified gurson and the modified mohrcoulomb fracture models over a wide range of stress triaxialities and lode angles, *Journal of the Mechanics and Physics of Solids* 59 (2011) 1374–1394.
- [31] L. Xue, Constitutive modeling of void shearing effect in ductile fracture of porous materials, *Engineering Fracture Mechanics* 75 (2008) 3343–3366.
- [32] L. E. Dhli, D. Morin, T. Brvik, O. S. Hopperstad, A lode-dependent gurson model motivated by unit cell analyses, *Engineering Fracture Mechanics* 190 (2018) 299–318.
- [33] A. U. Manual, Version 6.13-2, Dassault Systmes Simulia Corp., Providence, Rhode Island, USA (2013).
- [34] R. A. Oriani, The diffusion and trapping of hydrogen in steel, *Acta Metallurgica* 18 (1970) 147–157.
- [35] H. Yu, J. S. Olsen, J. He, Z. Zhang, Effects of loading path on the fracture loci in a 3D space, *Engineering Fracture Mechanics* 151 (2016) 22–36.
- [36] A. Gurson, Plastic flow and fracture behavior of ductile materials incorporating void nucleation, growth and coalescence, PhD Diss, Brown University (1975).

- [37] W. Jiang, Y. Li, J. Su, Modified gtn model for a broad range of stress states and application to ductile fracture, *European Journal of Mechanics - A/Solids* 57 (2016) 132–148.
- [38] Z. L. Zhang, Explicit consistent tangent moduli with a return mapping algorithm for pressure-dependent elastoplasticity models, *Computer Methods in Applied Mechanics and Engineering* 121 (1995) 29–44.
- [39] Z. L. Zhang, On the accuracies of numerical integration algorithms for gurson-based pressure-dependent elastoplastic constitutive models, *Computer Methods in Applied Mechanics and Engineering* 121 (1995) 15–28.
- [40] Z. L. Zhang, E. Niemi, A class of generalized mid-point algorithms for the gursontvergaard material model, *International Journal for Numerical Methods in Engineering* 38 (1995) 2033–2053.
- [41] R. Kiran, K. Khandelwal, Gurson model parameters for ductile fracture simulation in astm a992 steels, *Fatigue & Fracture of Engineering Materials & Structures* 37 (2014) 171–183.