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Numerical Simulation of Hydrogen Diffusion Coupled with Mechanical Loading using Abaqus/Standard and Abaqus/Explicit

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1. Introduction

1.1. Key Points of the Hydrogen Embrittlement Problem

The problem of hydrogen embrittlement in metals briefly consists in the following (Sofronis & McMeeking 1989, Taha & Sofronis 2001):

- Presence of atomic hydrogen in the lattice reduces the energy barrier for dislocation motion.
- As a result, macroscopic ductility is limited by highly localized plasticity.
- In the context of macroscopic modeling, one of the mechanisms proposed in HELP (Hydrogen Enhanced Localized Plasticity).

Hydrogen can be located:

- In normal interstitial lattice sites (NILS).
- In defects of the microstructure (dislocations, grain boundaries etc.).

For the numerical simulation of the phenomenon, user subroutines have been developed in both Abaqus Standard & Explicit (UMAT & VUMAT). The model has been tested in the problem of Mode-I fracture under small-scale yielding hypothesis.

1.2. Constitutive Modeling

For the solution of the coupled stress-diffusion constitutive model, an analogy between heat transfer & diffusion is being used (Barrera *et. al.* 2016, Diaz *et. al.* 2016):

	<u>Balance Equation</u>	<u>Flow Vector</u>
Heat Transfer:	$\rho \dot{U} + \nabla \cdot \mathbf{q} = \dot{r}$	$\mathbf{q}(\nabla T) = -\mathbf{k} \cdot \nabla T$
Hydrogen Diffusion:	$\dot{C}_L + \dot{C}_T + \nabla \cdot \mathbf{J} = 0$	$\mathbf{J}(\nabla C_L, C_L, \nabla p) = -D \nabla C_L + \dfrac{D V_H}{RT} C_L \nabla p$

<u>Analogy</u>

$T \rightarrow C_L$: Temperature $\rightarrow$ Lattice Hydrogen Concentration

$U \rightarrow C_{total}$: Internal Energy $\rightarrow$ Total Hydrogen Concentration

$\mathbf{q} \rightarrow \mathbf{J}$: Heat Flow $\rightarrow$ Hydrogen Flow

$\dot{r} \rightarrow 0$: Heat Source Term 0

For the implementation of the diffusion constitutive equations the UMATHT and VUMATHT user subroutines have been used in conjunction with UMAT and VUMAT subroutines (in Abaqus/Standard & Explicit respectively).

1.3. Example: Mode-I fracture under Small-Scale Yielding (SSY) conditions

In order to validate the codes that were developed, the problem of Mode-I fracture with small-scale yielding under plane strain has been addressed using both Abaqus/Standard and Abaqus/Explicit solvers.

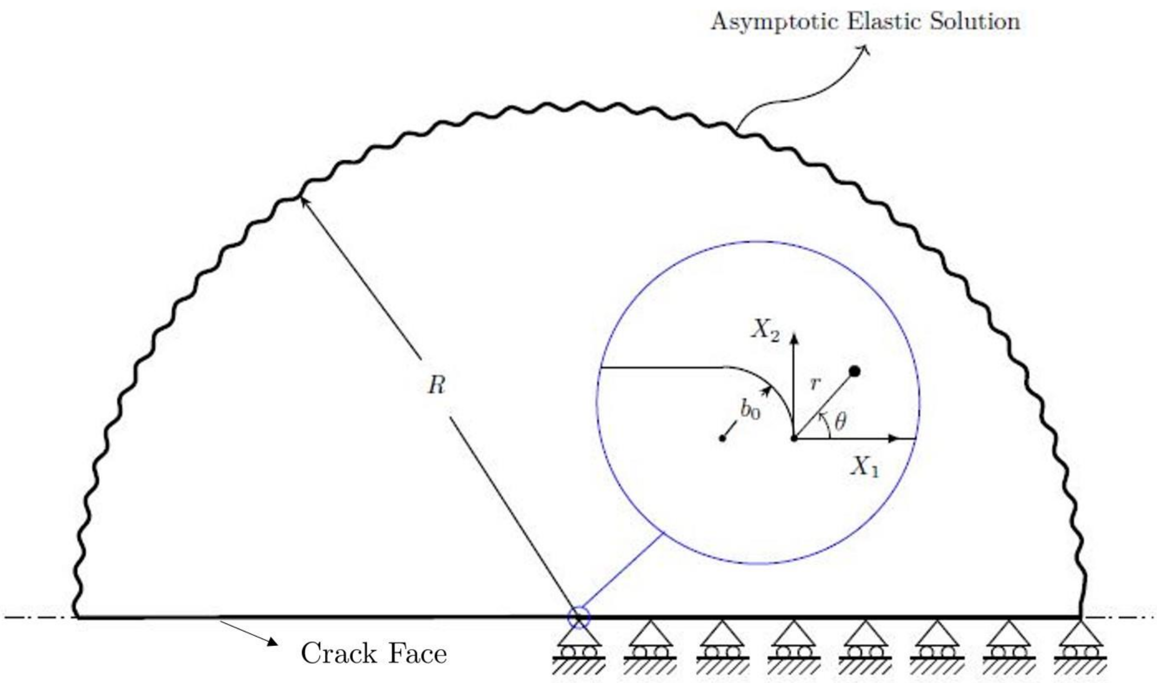


Figure 1: Schematic representation of geometry and boundary conditions near the crack tip for "small scale yielding" problem (R and b_0 is the initial notch size).

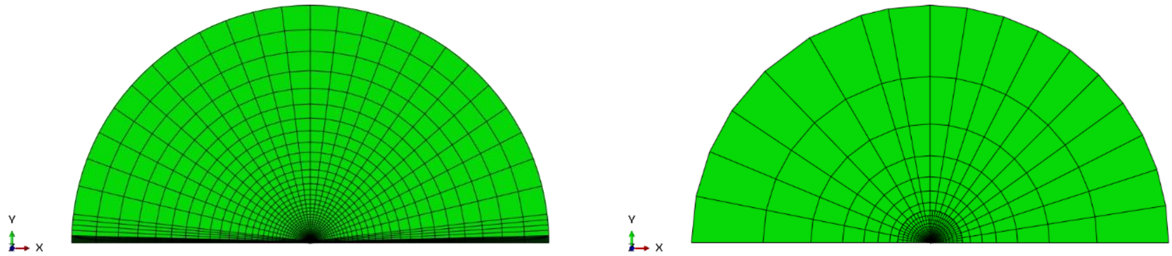
Traction free boundary conditions are used on the crack face and the elastic asymptotic mode-I displacement is imposed "far field" (e.g., see Aravas & Papadioti 2021):

$$\begin{Bmatrix} u_1^I \\ u_2^I \end{Bmatrix} = \frac{K_I}{2\mu}\sqrt{\frac{r}{2\pi}}\left(3-4\nu-\cos\theta\right)\begin{Bmatrix} \cos\dfrac{\theta}{2} \\ \sin\dfrac{\theta}{2} \end{Bmatrix}, \qquad K_I : \text{Stress Intensity factor}$$

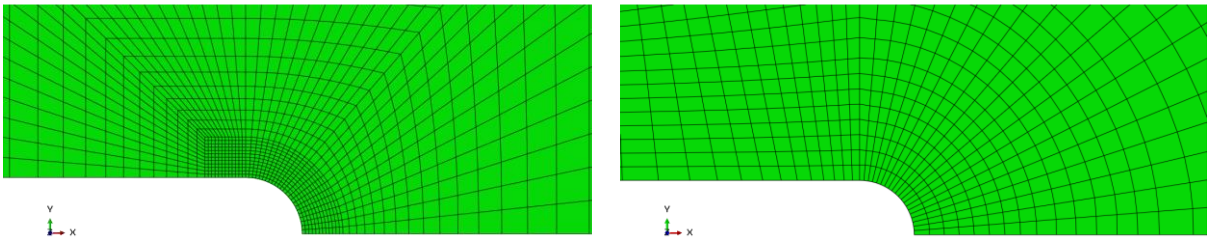
The finite element meshes used in the calculations are shown below.

Mesh 1 (Fine)
(Abaqus/Standard)

Mesh 2 (Coarse)
(Abaqus/Explicit)



overall mesh



crack tip detail

Mesh 1 (Fine):

- 6,134 8-node plane strain, coupled temperature-displacement elements (CPE8RT in ABAQUS/Standard)
- $R \approx 84 \times 10^3\, b_0$

Mesh 2 (Coarse):

- 1,658 4-node plane strain, coupled temperature-displacement elements (CPE4RT in ABAQUS/Explicit)
- $R \approx 1.2 \times 10^3\, b_0$

1.4. Properties and Normalization

The mechanical properties of the material and the properties related to hydrogen diffusion are summarized in Tables 1 and 2 (Taha & Sofronis, 2001):

Table 1: Mechanical properties

$E(GPa)$	ν	$\sigma_0(MPa)$	Hardening Exponent (n)
207	0.3	250	5

$$\sigma_y(\bar{\varepsilon}^p) = \sigma_0 \left(1 + \frac{\bar{\varepsilon}^p}{\varepsilon_0}\right)^{1/n}, \qquad \varepsilon_0 = \frac{\sigma_0}{E}$$

Table 2: Diffusion Properties

$D\left(\frac{m^2}{s}\right)$	$V_H\left(\frac{m^3}{mol}\right)$	K_T	$N_L\left(\frac{\text{Fe atoms}}{m^3}\right)$	λ	α	β
1.27×10^{-8}	2×10^{-6}	2.8×10^{10}	8.46×10^{28}	0.281	1	1

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Dimensions & material properties used in the input file are normalized as follows:

Dimensions & Time: $\hat{x}_i = \frac{x_i}{\ell}$, $\hat{u}_i = \frac{u_i}{\ell}$, $\hat{t} = \frac{t}{t_0}$

Mechanical Properties: $\hat{E} = \frac{E}{\sigma_0}$, $\hat{\sigma}_0 = \frac{\sigma_0}{\sigma_0} = 1$

Diffusion Properties: $\hat{C}_L = \frac{C_L}{C_0}$, $\hat{N}_L = \frac{N_L}{C_0}$, $\hat{D} = \frac{D}{\ell^2 / t_0}$, $\hat{V}_H = \frac{V_H}{RT/\sigma_0}$

Loads: $\hat{K}_I = \frac{K_I}{\sigma_0\sqrt{\ell}}$

Table 3: Normalizing Parameters

$\ell(\mathrm{m})$	$t_0(\mathrm{s})$	$C_0\left(\frac{\text{H atoms}}{\mathrm{m}^3}\right)$	$R\left(\frac{\mathrm{J}}{\mathrm{mol}\times\mathrm{K}}\right)$	$T(\mathrm{K})$
5×10^{-6}	1	2.086×10^{21}	8.314	300

2. Simulations using Abaqus/Standard

Comparison was carried out with the predictions of Taha & Sofronis (2001) and good agreement was found. The loads and boundary conditions imposed are summarized in Table 4. The results are shown in Figures 2-7 below.

Table 4: Loads and boundary conditions for the mode-I fracture problem with hydrogen diffusion (Taha & Sofronis, 2001).

Load Level (K_I)	$89.7\ \mathrm{MPa}\sqrt{\mathrm{m}}$
Total Time	130 s
Constant Concentration B.C.	$C_L^{\text{Crack Face}} = C_0$
Zero Flux B.C.	$\mathbf{J}^{\text{Crack Face}} = \mathbf{0}$

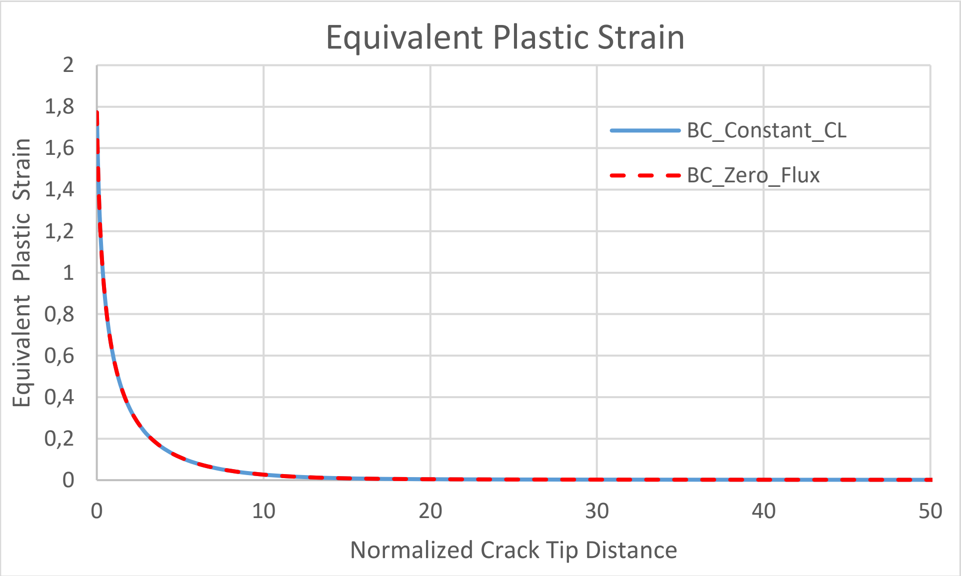

Figure 2: Distribution of $\bar{\varepsilon}^p$ near the crack tip.

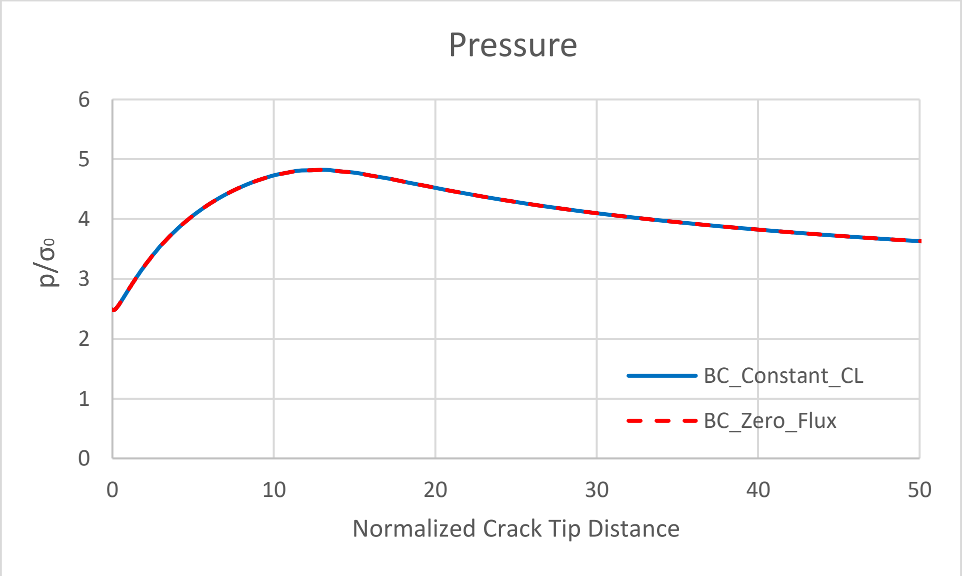

Figure 3: Distribution of normalized pressure near the crack tip.

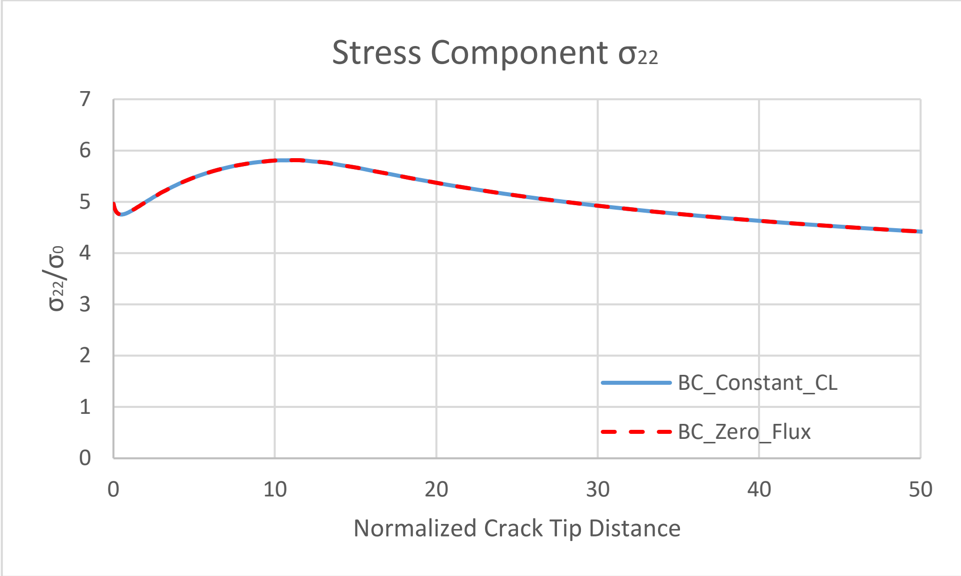

Figure 4: Distribution of normalized stress in the direction of loading near the crack tip.

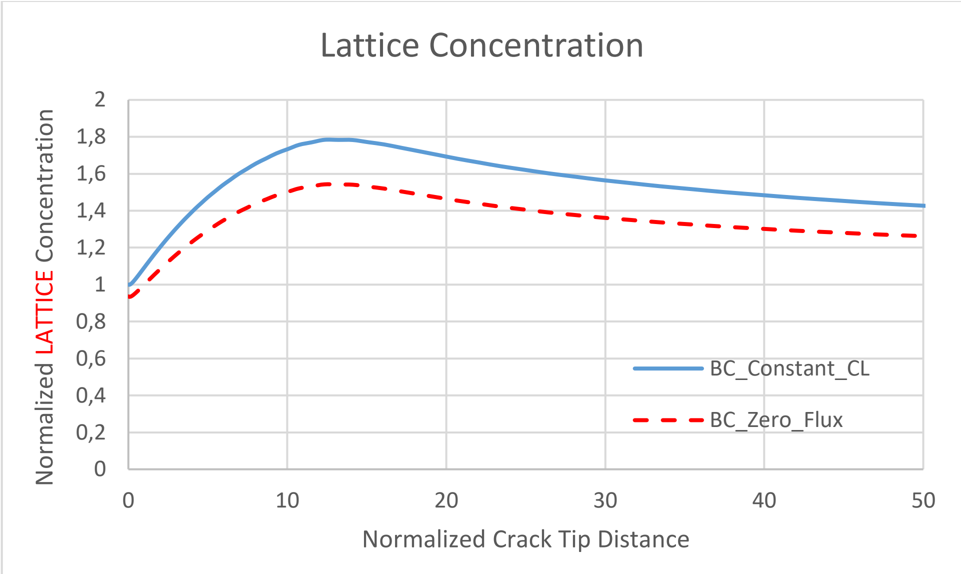

Figure 5: Distribution of normalized lattice concentration C_L / C_0 near the crack tip.

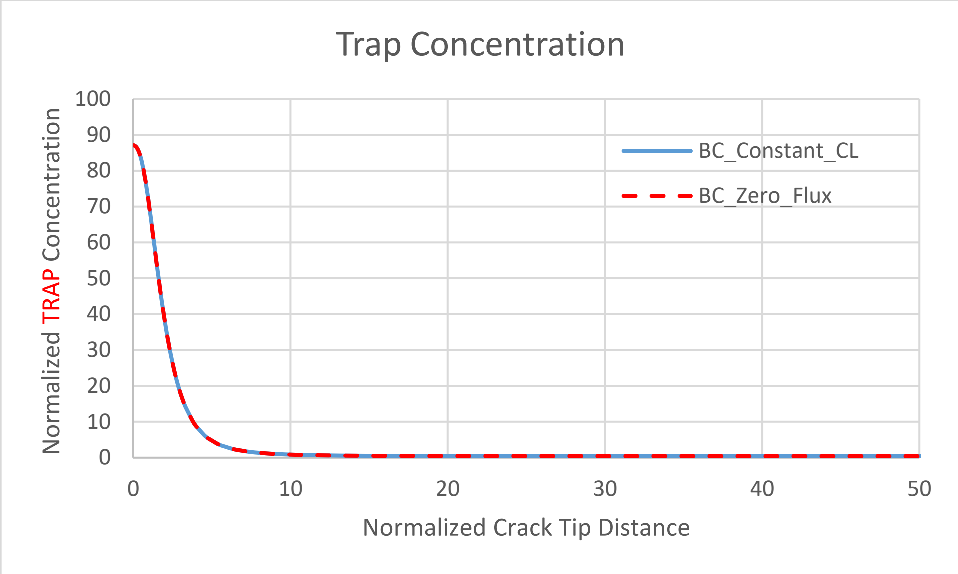

Figure 6: Distribution of normalized trap concentration C_T / C_0 near the crack tip.

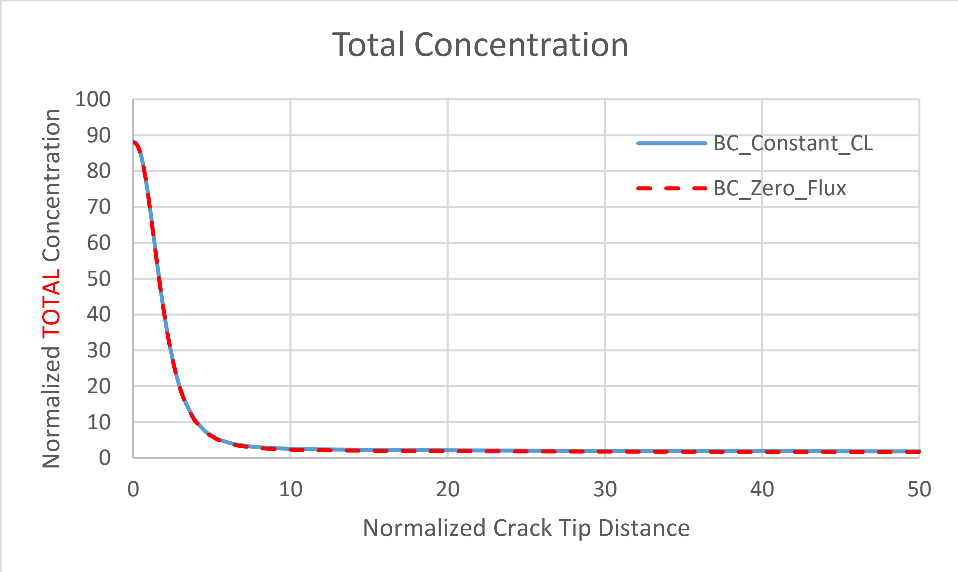

Figure 7: Distribution of normalized total concentration $(C_L + C_T)/C_0$ near the crack tip.

3. Simulations using Abaqus/Explicit

The problem of Mode-I fracture under plane strain with small-scale yielding has been simulated by using Abaqus/Explicit. In this case, 4-node bilinear elements with reduced integration have been used. Details for the calculations are summarized in Table 5[1].

Both 2D and 3D (with appropriate boundary conditions) simulations have been performed and the results are shown to be in good agreement with those predicted using Abaqus/Standard. *The small difference in the predicted values at the tip of the notch are due to the much finer mesh used in ABAQUS/Standard*.

Table 5: Loads and boundary conditions for the mode-I fracture problem with hydrogen in Abaqus/Explicit.

Load Level (K_I)	$22.425\ \mathrm{MPa}\sqrt{\mathrm{m}}$
Total Time	32.5 s
Zero Flux B.C.	$\mathbf{J}^{\text{Crack Face}} = \mathbf{0}$

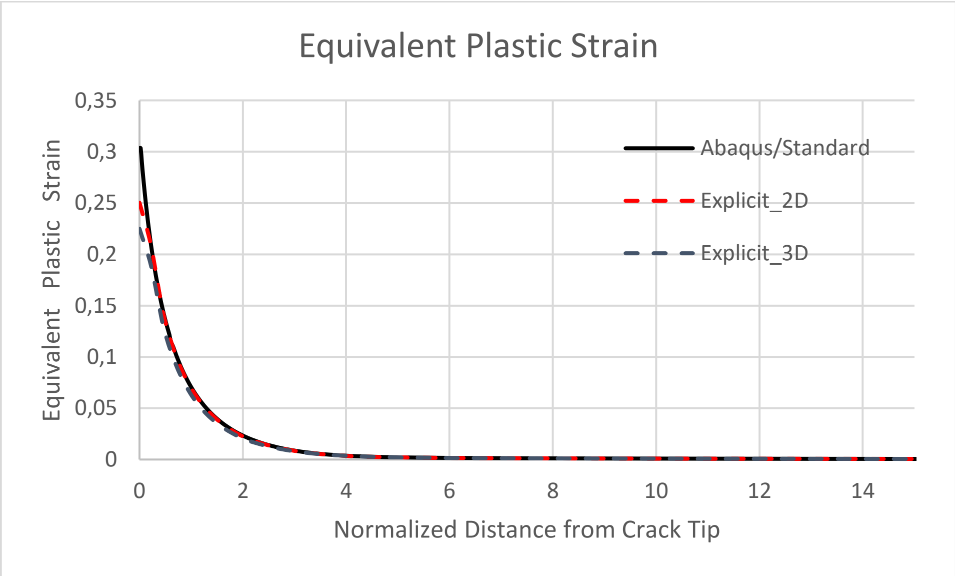

Figure 8: Distribution of $\bar{\varepsilon}^p$ near the crack tip.

[1] Simulations using Abaqus/Explicit are by default dynamic (i.e., inertia forces are included in the calculations). For the simulations to be equivalent to the ones with Abaqus/Standard (*STATIC), density ρ is chosen so that the kinetic energy is no more than 5% of the strain energy at the end of the analysis.

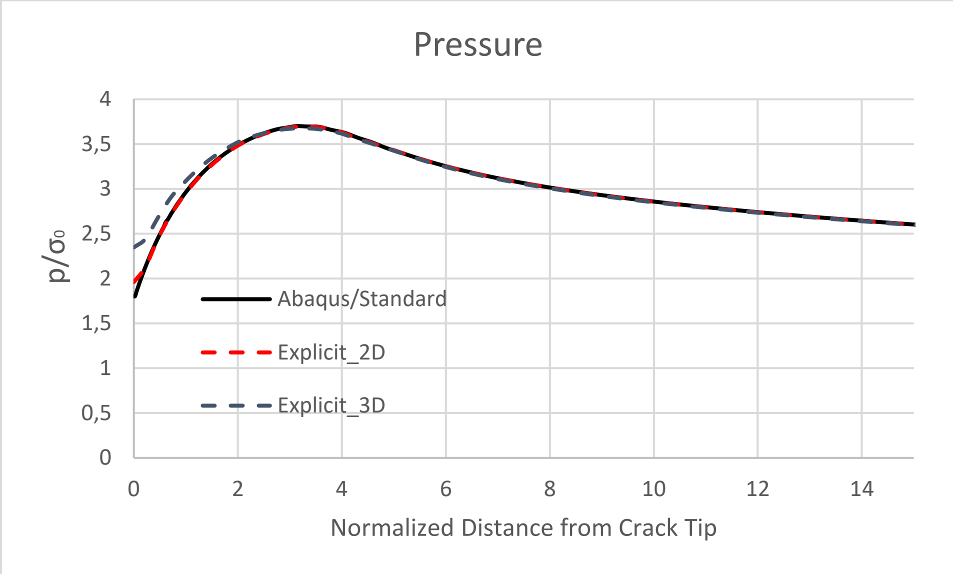

Figure 9: Distribution of normalized pressure near the crack tip.

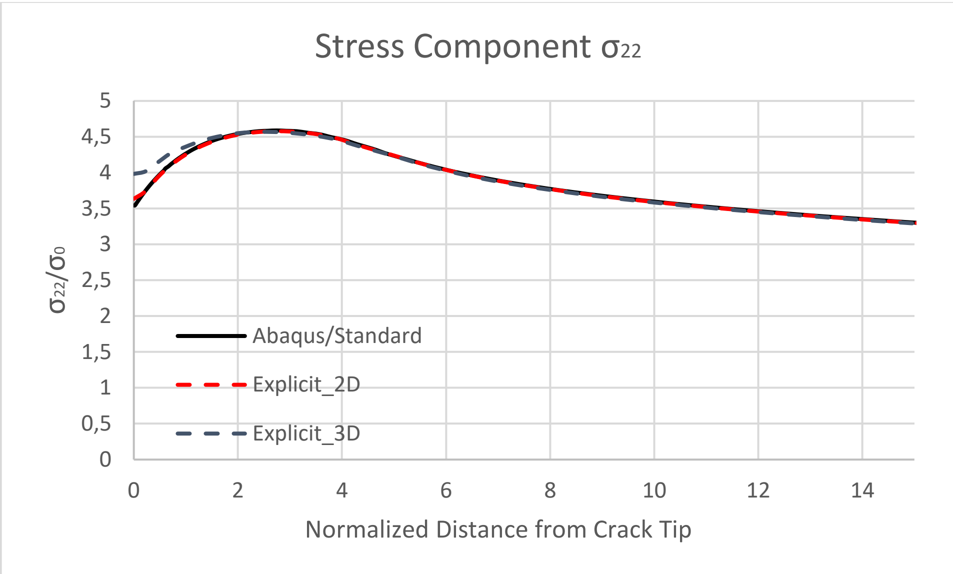

Figure 10: Distribution of normalized stress in the direction of loading near the crack tip.

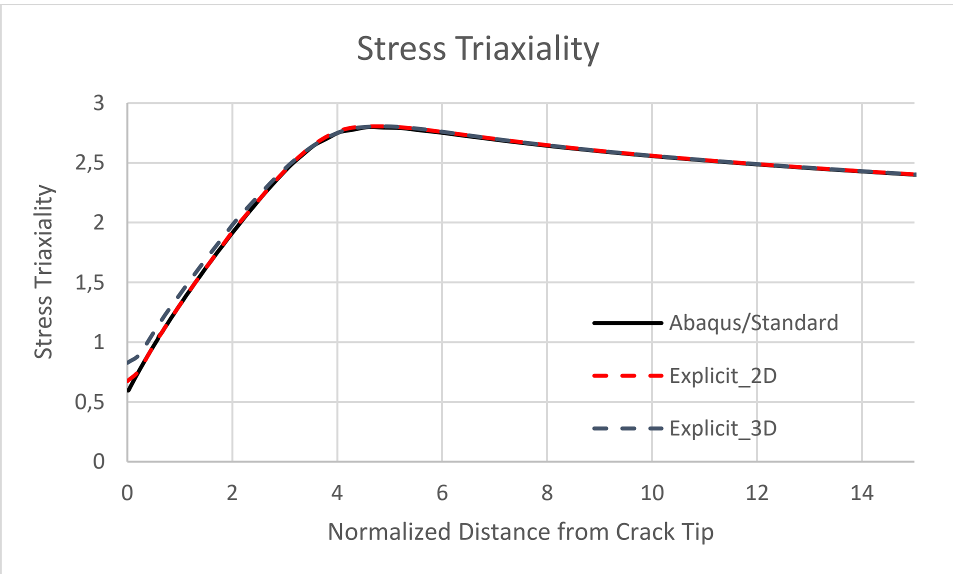

Figure 11: Distribution of stress triaxiality X_{Σ} near the crack tip.

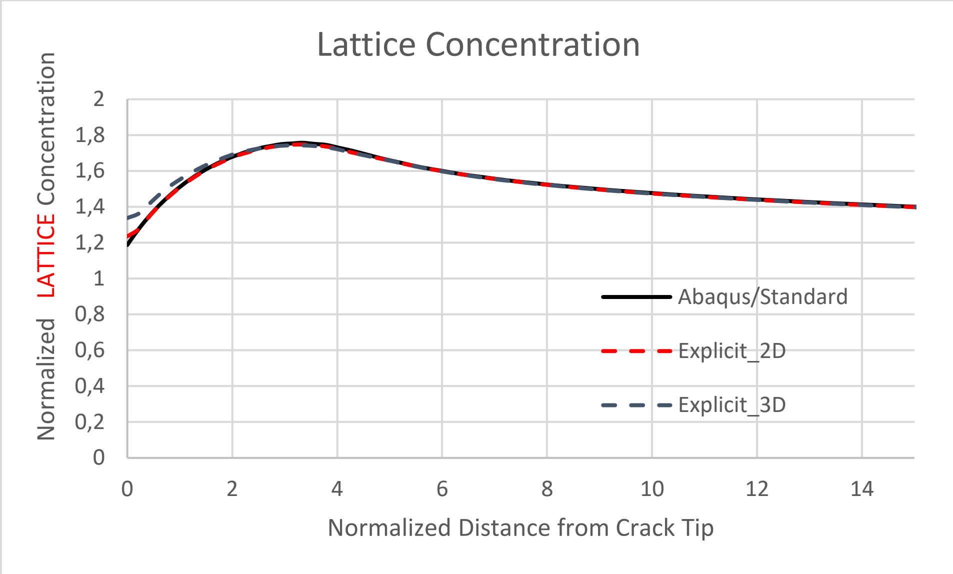

Figure 12: Distribution of normalized lattice concentration C_L / C_0 near the crack tip.

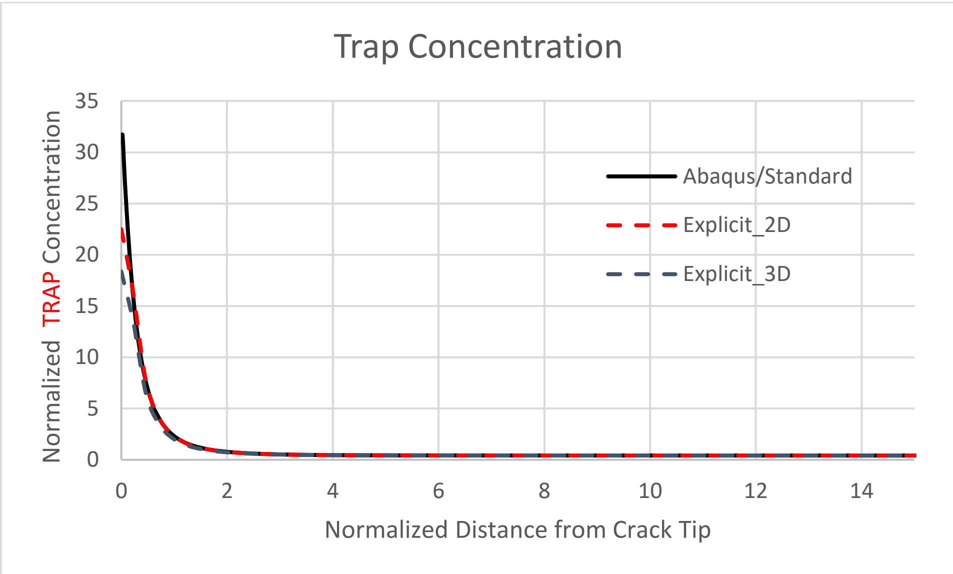

Figure 13: Distribution of normalized trap concentration C_T / C_0 near the crack tip.

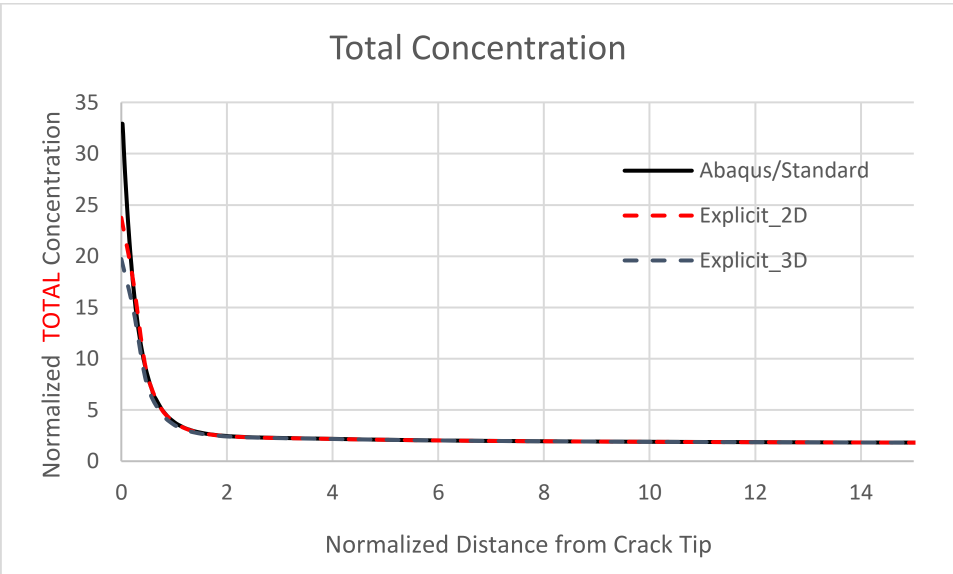

Figure 14: Distribution of normalized total concentration $(C_L + C_T)/C_0$ near the crack tip.

4. References

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Sofronis, P., McMeeking, R.M., 1989. Numerical analysis of hydrogen transport near a blunting crack tip. *J. Mech. Phys. Solids* **37(3)**, 317-350.

Taha, A., Sofronis, P., 2001. A micromechanics approach to the study of hydrogen transport and embrittlement. *Eng. Fract. Mech.* **68**, 803-837.