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Reconsideration of the Hydrogen Diffusion Model Using the McNabb-Foster Formulation

by

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Abstract

In the current paper, instead of the Oriani formulation used by Sofronis and McMeeking, a more general formulation introduced by McNabb and Foster is adopted and applied successfully to a non-symmetric hydrogen diffusion scheme. The results are compared to Sofronis and McMeeking's and Krom et al.'s work for the hydrogen diffusion near a blunting crack tip. Results represent that the McNabb-Foster formulation produces drastically different hydrogen distribution from Oriani's equilibrium theory in both trap and lattice sites particularly when the loading time is significantly small.

Keywords: Hydrogen embrittlement, Trapping, Crack, Equilibrium theory, Advection diffusion, Finite element

1. Introduction

Hydrogen embrittlement is a common type of failure^{1,2)}. In presence of hydrogen, materials fail at a lower load level in comparison to hydrogen-free materials. Hydrogen-enhanced localized plasticity (HELP) is an acceptable mechanism of hydrogen embrittlement and hydrogen-induced cracking in materials³⁻⁵⁾. According to the HELP theory, the presence of hydrogen in a solid solution increases the dislocation motion, thereby increasing the amount of plastic deformation that occurs in a localized region adjacent to the fracture zone.

A possible way by which the HELP mechanism can bring about macroscopic material failure is through hydrogen-induced cracking. The fracture and fatigue behavior of a cracked plate under external load depends upon the stress and strain in the vicinity of the crack tip. Sofronis and McMeeking⁶⁾ proposed a finite element model to show the effect of hydrostatic stress and trapping phenomenon on hydrogen distribution in plastically deformed steels. Based on their model, Krom

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et al. ⁷⁾ suggested a formulation to provide the correct balance of hydrogen into the considered material by applying the strain rate term to the advection diffusion equation. Kanayama et al. ⁸⁾ used a different finite element scheme from Krom et al. ⁷⁾ and applied the Galerkin method in a 3D simulation in order to reconstruct the Sofronis and McMeeking's model ⁶⁾.

Sofronis ⁹⁾ applied and compared the Oriani's equilibrium theory ¹⁰⁾ with the McNabb-Foster formulation ¹¹⁾ in a "hydrogen diffusion near a crack tip" problem. In our previous articles ^{8,12)}, Sofronis and McMeeking's model has been studied and a stabilized method was developed. One of the conclusions of Sofronis ⁹⁾ is that both methods provide satisfying results; therefore, the Oriani's equilibrium theory which is simpler than the McNabb-Foster formulation is enough to solve the considered hydrogen diffusion problem. The problem in the abovementioned statement is that the Oriani's equilibrium theory is clearly based on the hydrogen distribution in lattice sites and the trap site concentration is determined as a function of the lattice site concentration. As it is shown in the current paper, the McNabb-Foster formulation is actually more suitable when it is considered to study the hydrogen concentration in trap sites. In their work ¹¹⁾, McNabb and Foster questioned the validity of the Fick's laws and their associated physical model of non-interacting particles in random motion through the medium and also suggested a mathematical model that should be able to correct the anomalies noticed in the Fick's laws. The McNabb-Foster formulation assumes that hydrogen diffuses through the crystal lattice in accordance with the first Fick's law.

Let us consider θ_T as the occupancy of trap sites. The number of hydrogen atoms released in a unit volume δV by active trap sites is given by

$$N_1 = p\theta_T N_T \delta V \quad (1)$$

where N_T is the number of trap sites per unit volume and p represents the "probability" that a trap site containing a hydrogen atom releases it before one second has passed. On the other side, the number of hydrogen atoms captured by the active trap sites in a unit volume δV is

$$N_2 = kC_L(1-\theta_T)N_T \delta V \quad (2)$$

where the parameter k represents the "probability" that a trap site will capture hydrogen atoms. The flux of hydrogen atoms through a bounded surface S of an arbitrary volume V of an isotropic homogeneous medium containing N_T trap sites per unit volume is now considered. The diffusing lattice site hydrogen concentration is defined by C_L . The following partial differential equation is presented in McNabb and Foster's work ¹¹⁾

$$\frac{\partial C_L}{\partial t} + N_T \frac{\partial \theta_T}{\partial t} = \nabla \cdot (D_L \nabla C_L). \quad (3)$$

An important remark is that the trap site number per unit volume N_T is assumed as a constant in the model originally considered by McNabb and Foster ¹¹⁾. Finally, for a unit volume δV , the rate of increase of the number of atoms in the trapped population $\partial(\theta_T N_T \delta V)/\partial t$ is equivalent to the difference between the rates of capture and release:

$$\frac{\partial \theta_T}{\partial t} = kC_L(1-\theta_T) - p\theta_T. \quad (4)$$

One can see how the McNabb-Foster formulation is more suitable to analyze the trap data. The trap site concentration is not a direct function of the lattice concentration as it is the case in the Oriani's equilibrium theory. It is also very important to notice that unlike the Oriani's theory, the McNabb-Foster formulation is not limited to the equilibrium state between trap sites and lattice sites.

If a steady case is considered, then the following relation can be deduced from Eq. (4):

$$\frac{k}{p} C_L = \frac{\theta_T}{(1-\theta_T)}. \quad (5)$$

Using the following relation

$$\theta_T = \frac{1}{1 + \frac{N_L}{K_T C_L}} = \frac{K_T C_L}{K_T C_L + N_L} \quad (6)$$

which is based on the Oriani's assumption ¹⁰⁾ and was applied in our previous work ⁸⁾ where $K_T = e^{-\Delta E_T/RT}$ and N_L is the number of lattice sites per unit volume, a relation between the parameters k and p can finally be found as follows:

$$\frac{k}{p} = \frac{\exp(-\Delta E_T/RT)}{N_L}. \quad (7)$$

Krom in his thesis paper ¹³⁾ also applied both the McNabb-Foster and the Oriani formulations to his improved version of Sofronis and McMeeking's studies. Though, in the improved version, the hydrogen concentration in lattice sites is modified, Krom et al.⁷⁾ and Sofronis ⁹⁾ still consider the Oriani's equilibrium theory as sufficient to solve the advection diffusion problem. In the previous studies ^{8,12)}, we modified the numerical scheme used in the Krom's work with the objective of adding a stabilization term. In the current work, the McNabb-Foster formulation is considered for the modified model based on Krom's study. The intent of the current paper is to represent that the McNabb-Foster formulation produces drastically different results from Oriani's equilibrium theory when it is assumed to study the hydrogen concentration in both trap and lattice sites particularly in a significantly small loading time.

2. Hydrogen Diffusion Model by the McNabb-Foster Formulation

Using the Sofronis and McMeeking's model presented in **Fig. 1**, a semi-circular body with a volume Ω and a surface $\partial\Omega = \Gamma$ is considered. Constants C_b and C_{L0} are given numbers of hydrogen atoms per unit volume in lattice sites. J is the hydrogen flux, u_i is the displacement components and T is the traction vector. Detailed explanations of the structural analysis and the related formulations can be found in the reference (14). According to the mass conservation law, the changing rate of the total hydrogen in the volume Ω is equivalent to the flux through Γ as follows:

$$\frac{\partial}{\partial t} \int_{\Omega} (C_L + C_T) d\Omega + \int_{\partial\Omega} J \cdot n ds = 0, \quad (8)$$

$$J = -M_L C_L \nabla \mu_L \quad \text{and} \quad \mu_L = \mu_L^0 + RT \log_e \frac{C_L}{N_L} - \bar{V}_H \sigma_h.$$

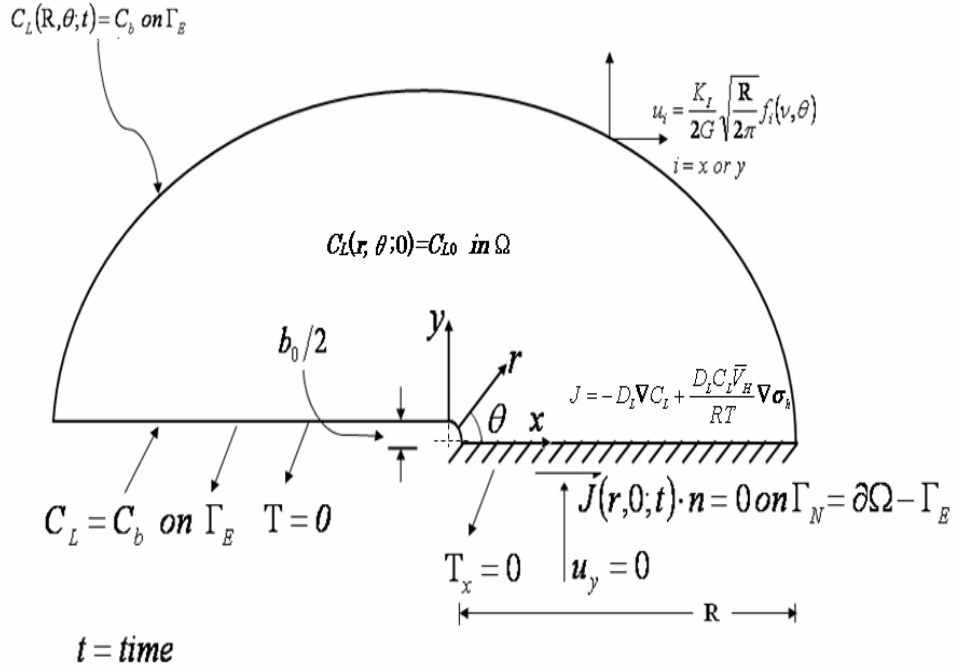


Fig. 1 Description of the boundary and initial conditions for the one side coupled diffusion and elasto-plastic problem under small scale yielding conditions ⁶⁾.

C_L and C_T are respectively the number of hydrogen atoms per unit volume in lattice sites and in trap sites. n is the outward normal vector, M_L is the mobility of the hydrogen in the lattice sites, N_L is the number of lattice sites per unit volume, and μ_L is the chemical potential in lattice sites. R is the gas constant, T is the absolute temperature, μ_L^0 is the chemical potential at a reference

temperature and pressure, and σ_h is defined as the hydrostatic stress such that $\sigma_h = \frac{1}{3} \sum_{i=1}^3 \sigma_{ii}$

where σ_{ii} is the stress tensor components. \bar{V}_H is the partial molar volume of hydrogen. Using

the expression of μ_L , the hydrogen flux can be expressed by the lattice diffusivity D_L as

$$J = -D_L \nabla C_L + \frac{C_L D_L \bar{V}_H}{RT} \nabla \sigma_h, \quad D_L = M_L RT. \quad (9)$$

After substituting Eq. (9) into Eq. (8) and applying the divergence theorem, the obtained formulation for the arbitrary volume Ω is

$$\frac{\partial C_L}{\partial t} + \frac{\partial C_T}{\partial t} - \nabla \cdot (D_L \nabla C_L) + \nabla \cdot \left(\frac{C_L D_L \bar{V}_H}{RT} \nabla \sigma_h \right) = 0. \quad (10)$$

The trap site concentration can be related to the number of sites as follows:

$$C_T = \theta_T N_T. \quad (11)$$

Combining Eq. (10) and Eq. (11), the following equation can be easily deduced:

$$\frac{\partial C_L}{\partial t} + N_T \frac{\partial \theta_T}{\partial t} - \nabla \cdot (D_L \nabla C_L) + \nabla \cdot \left(\frac{C_L D_L \bar{V}_H}{RT} \nabla \sigma_h \right) + \theta_T \frac{dN_T}{d\varepsilon_p} \frac{\partial \varepsilon_p}{\partial t} = 0. \quad (12)$$

In the equation considered by Krom et al. ⁷⁾, the number of trap sites per unit volume N_T is not constant. The new hydrogen diffusion equation consists of a combination of Eqs. (4) and (12). Equation (7) is used for the choice of the parameters k and p . After writing the weak form of Eq. (12) as follows:

$$\begin{aligned} & \left(\frac{\partial C_L}{\partial t}, C_L^* \right) + \left(N_T \frac{\partial \theta_T}{\partial t}, C_L^* \right) + (D_L \nabla C_L, \nabla C_L^*) - \left(\frac{C_L D_L \bar{V}_H}{RT} \nabla \sigma_h, \nabla C_L^* \right) \\ & + \left(\theta_T \frac{dN_T}{d\varepsilon_p} \frac{\partial \varepsilon_p}{\partial t}, C_L^* \right) = 0 \end{aligned} \quad (13)$$

where $(A, B) = \int A \cdot B d\Omega$ (see the reference (8) for more details) and C_L^* is a test function, the

finite difference in time of Eq. (13) accompanied by considering the equation^{6,7)}

$$\log_{10}(N_T) = 23.26 - 2.33 e^{-5.5\varepsilon_p} \text{ produces}$$

$$\begin{aligned} & \left(\frac{C_L^{n+1} - C_L^n}{\Delta t}, C_L^* \right) + \left(N_T^n \frac{\theta_T^{n+1} - \theta_T^n}{\Delta t}, C_L^* \right) + (D_L \nabla C_L^{n+1}, \nabla C_L^*) \\ & - \left(\frac{C_L^{n+1} D_L \bar{V}_H}{RT} \nabla \sigma_h, \nabla C_L^* \right) + \left(\theta_T^n 29.508 N_T (\varepsilon_p^n) e^{-5.5\varepsilon_p^n} \left(\frac{\varepsilon_p^{n+1} - \varepsilon_p^n}{\Delta t} \right), C_L^* \right) = 0. \end{aligned} \quad (14)$$

It should be mentioned that an implicit method is used for Eq. (14) and following the pioneers ^{6,7,9)}, because of an excellent stability character in the sense of the maximum norm, the backward time difference is adopted for the abovementioned equation.

A finite difference method using an explicit Euler scheme is implemented to solve Eq. (4), and the result is added into Eq. (14). It is worth to mention here that because of applying an explicit scheme, a smaller time increment τ is used instead of Δt in the resolution of Eq. (4) as it can be observed in Eq. (15):

$$\frac{\theta_T^{n+\frac{1}{m}} - \theta_T^n}{\tau} = kC_L^n(1 - \theta_T^n) - p\theta_T^n. \quad (15)$$

$(\Delta t = m\tau, m > 1)$

The main motivation in the choice of a different time increment for Eq. (15) is mainly to improve the result precision provided by the finite difference method. Unlike the current paper, Sofronis⁹⁾ implemented an implicit backward time difference to solve Eq. (4).

3. Numerical Specifications

The finite element analyses are here employed to solve the boundary value problems of large strain elastoplasticity-transient hydrogen diffusion in the vicinity of a blunting crack tip under mode I (tensile) opening and small scale yielding conditions¹⁴⁾. **Figure 1** shows the half-symmetry 3D geometry domain and the boundary conditions used for structural and diffusion analysis. As mentioned in this figure, symmetry boundary conditions are applied on the crack plane $y=0$ while the displacements through the thickness are completely constrained ($u_z=0$). The symmetry line $\theta = 0$ is free of shear tractions and the displacements in the y direction are constrained ($u_y=0$) while on the disc circumference, the displacements are known from the elastic solution, which is controlled by K_I (see reference (14) for more details). The load is increasing from zero at a rate of $0.69 \text{ MPa(m)}^{0.5}\text{s}^{-1}$ for 130 s with steps of 0.5 s. The mesh consists of 10,656 nodes and 3,706 10-node tetrahedral elements. It is refined near the crack tip (see **Fig. 2**). The model dimensions, analysis specifications and constant values can respectively be found in the **Table 1**, **Table 2** and **Table 3**.

Table 1 Model dimensions.

| | | |
|---------------------------|----------|---------------------------|
| Initial crack tip opening | b_0 | $1.0 \times 10^{-5} [m]$ |
| Model radius | R | $1.5 \times 10^{-1} [m]$ |
| Model thickness | h | $8.25 \times 10^{-4} [m]$ |

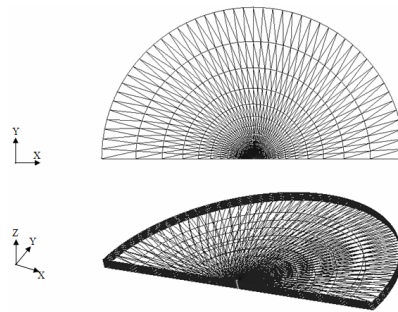


Fig. 2 The 3D mesh including the tetrahedral elements.

Table 2 Analysis specifications.

| | |
|---|---------------------------------|
| Number of elements | 3,706 |
| Number of nodes | 10,656 |
| CPU | Pentium 4 3.2 GHz |
| Memory | 2.0 GB |
| CPU time | 480-600[s] |
| Time increment Δt | 0.005[s], 0.5 [s], etc... |
| Total time | 1.3[s], 130[s], etc... |
| Number of total steps | 260 |
| Solver | BiCGSTAB(L); L=4 Ref. (15) |
| Preconditionner | Shifted ILU (shift value: 1.05) |
| Convergence criterion for relative residuals in BiCGSTAB (L). | 10^{-6} |

Table 3 Constant values and material properties ^{6,7,8}.

| | | |
|----------------------------------|--------------|--|
| Diffusion constant | D_L | $1.27 \times 10^{-8} [m^2 \cdot s^{-1}]$ |
| Gas constant | R | $8.3144 [J \cdot mol^{-1} \cdot K^{-1}]$ |
| Temperature | T | $300 [K]$ |
| Initial hydrogen concentration | C_{L0} | $2.08 \times 10^{21} [m^{-3}]$ |
| Partial molar volume of hydrogen | \bar{V}_H | $2 \times 10^{-6} [m^3 \cdot mol^{-1}]$ |
| Lattice sites per unit volume | N_L | $5.10 \times 10^{29} [m^{-3}]$ |
| Trap binding energy | ΔE_T | $-60 \times 10^3 [J \cdot mol^{-1}]$ |
| Poisson ratio | ν | 0.3[-] |
| Young modulus | E | 207[GPa] |
| Yield stress | σ_y | 250[MPa] |

4. Results

In **Fig. 3**, The hydrogen distribution in lattice sites at 130[s] along the symmetry line $\theta = 0$ concluded from our analysis considering the McNabb-Foster formulation has been compared with Krom et al.'s results ⁷ using Oriani's equilibrium theory. The results with the strain rate factor and without the strain rate factor are computed considering the McNabb-Foster formulation for a loading time of 130[s]. **Fig. 3** illustrates that for the initial value of $\theta_{T0} = 9.914 \times 10^{-1}$ considered by Sofronis and McMeeking ⁶, the result obtained by the McNabb-Foster formulation adding the plastic strain rate is slightly higher than the result obtained by Krom et al. with the Oriani formulation. The obtained result by considering the parameters of Sofronis's thesis paper confirms the influence of the plastic strain rate introduced by Krom et al. even in the reconsidered equation using the McNabb-Foster formulation (see Fig. 4 of Krom et al. ⁷ for the effect of plastic strain rate while applying the Oriani formulation). In Eq. (15), for the case of $\Delta t = 0.5 [s]$, m is chosen 1,000 that means the second time increment $\tau = 5 \times 10^{-4} [s]$ (see Eq. (15)). In other words, using an explicite Euler scheme for Eq. (4), 1000 iterations are needed

in Eq. (15) to calculate the trap site occupancy θ^{n+1} precisely, which is then used in the main Eq. (14). C_{L0} is the initial hydrogen concentration in the whole model including the symmetry line ($\theta = 0^\circ$).

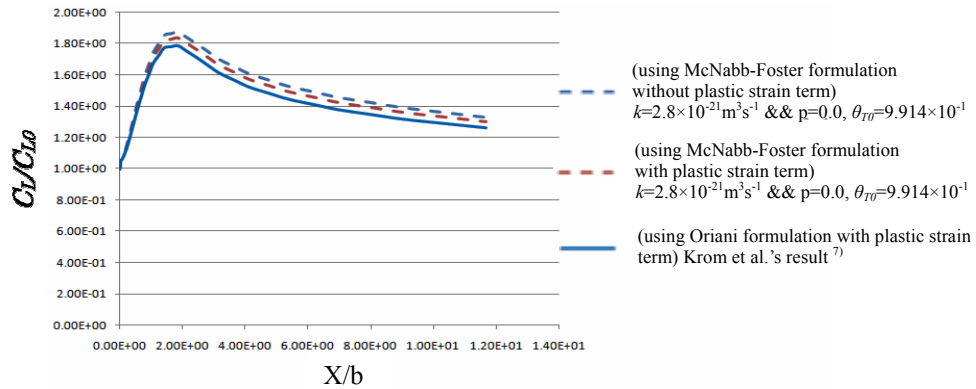


Fig. 3 Comparison of the hydrogen distribution near the crack tip between Oriani and McNabb-Foster formulations for a loading time of 130 s ($b = 4.7 b_0$ and X is the distance of the initial position of each node from the notch root in the undeformed configuration.)

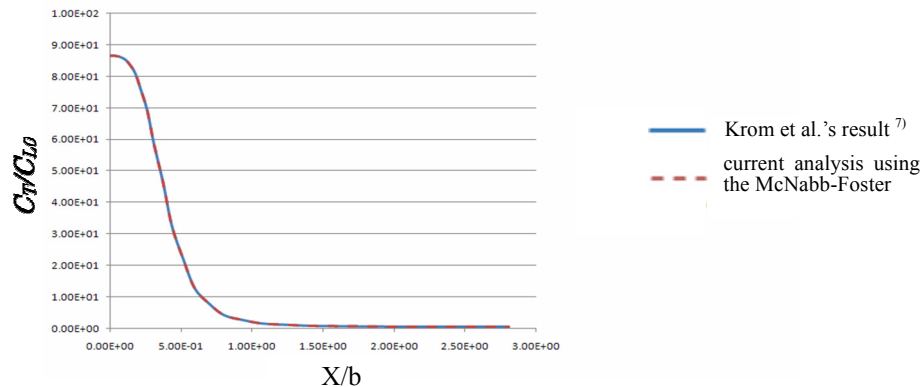


Fig. 4 Hydrogen diffusion near the crack tip in trap sites using the McNabb-Foster formulation for a loading time of 130 s ($k=2.8 \times 10^{-21} \text{m}^3 \text{s}^{-1}$, $b = 4.7 b_0$ and X is the distance of the initial position of each node from the notch root in the undeformed configuration.)

Krom et al.'s results⁷⁾ for hydrogen distribution in trap sites are also compared with the current results using the McNabb-Foster formulation in **Fig. 4** for a loading time of 130 s. As can be seen in **Fig. 4**, for the loading time of 130 seconds, the results produced by the McNabb-Foster formulation generally show a good agreement with other studies^{6,7,8)} using the equilibrium theory established by Oriani¹⁰⁾. However, different results of hydrogen distribution in lattice sites and trap sites are observed for the loading times lower than 130 seconds. The hydrogen distribution in trap sites using the McNabb-Foster formulation has been computed for different loading times in **Fig. 5**. Unlike Krom et al.'s results presented in Fig. 7 of their paper, the observed results in **Fig. 5** show that we have lower hydrogen concentration in trap sites for smaller loading times. In the one-dimensional analysis, Krom¹³⁾ mentions that by increasing the plastic strain rate (decreasing

the loading time), the hydrogen concentration deviates from the equilibrium concentration assumed by the Oriani's theory. In other words, the local equilibrium between hydrogen concentration in lattice sites and trap sites can only be assumed for the certain level of the plastic strain rate lower than 0.1 s^{-1} ¹³⁾ in the one-dimensional analysis. It is in an qualitatively agreement with the different results obtained here by using the McNabb-Foster formulation compared to the results obtained by Krom et al. using the Oriani formulation. The derivation of the computed level of the critical plastic strain rate in the two-dimensional case of the current model is shown in subsequent paragraph.

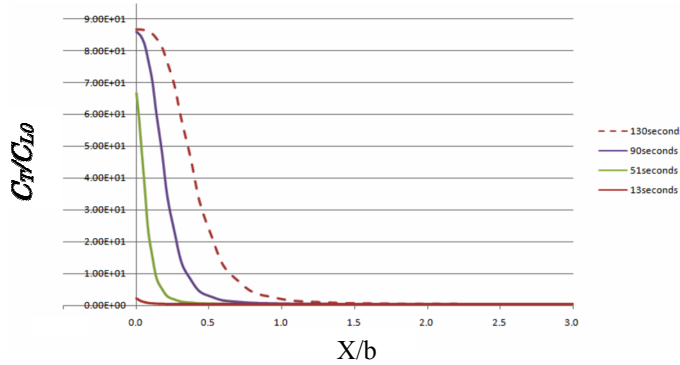


Fig. 5 The effect of the loading time on the hydrogen concentration distribution in trap sites near the crack tip using the McNabb-Foster formulation ($k=2.8 \times 10^{-21} \text{ m}^3 \text{ s}^{-1}$).

Using the McNabb-Foster formulation, the hydrogen distribution in lattice sites has been plotted for different loading times in **Fig. 6**. Comparing **Fig. 6** with Fig. 6 of Krom et al. ⁷⁾ which illustrates the results for different loading time in the case of using the Oriani's theory, abovementioned results are completely different from the previous study ⁷⁾. A horizontal asymptote appears for the ratio of hydrogen concentration over the initial concentration in lattice sites. Thus, the concentration in lattice sites never goes below the mentioned asymptote in the McNabb-Foster formulation.

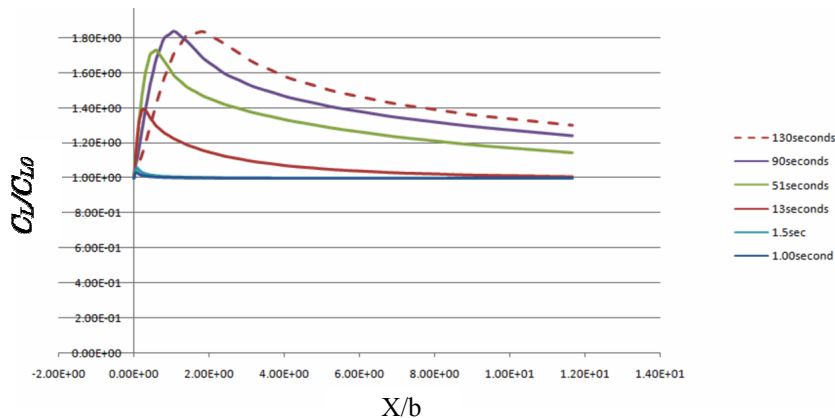


Fig. 6 Influence of the loading time on the hydrogen concentration distribution in lattice sites near the crack tip, using the McNabb-Foster formulation for several loading times ($k=2.8 \times 10^{-21} \text{ m}^3 \text{ s}^{-1}$).

Figures 7 and 8 extend the results of the normalized lattice concentration for sufficiently long loading time by using respectively the Oriani's equilibrium theory and the McNabb-Foster formulation. **Figure 9** shows the normalized trap concentration for the sufficiently long loading

time in the case of using the McNabb-Foster formulation. As can be seen in **Figs. 7, 8 and 9**, if the loading time increases over 130s, the results show a good agreement between the Oriani's equilibrium theory and the McNabb-Foster formulation. These results confirm the fact that for the sufficiently long loading times, the trapping of hydrogen can be assumed as a function of lattice concentration as it is the case in the Oriani's equilibrium theory. As it is explained before, according to Krom¹³⁾ for the one-dimensional analysis, the local equilibrium between hydrogen concentration in lattice sites and trap sites can only be assumed for the certain level of the plastic strain rate lower than 0.1 s^{-1} . In our two-dimensional analysis, according to **Fig. 9**, the computed level of the required time for attaining the steady state situation in trap sites is almost 130[s]. According to references (6) and (14), the value of the plastic strain at the crack tip vicinity for the same model is almost 1.4, which requires the plastic strain rate of the level 0.01 s^{-1} where both McNabb-Foster and Oriani formulations produce the same results (see also **Fig. 4**).

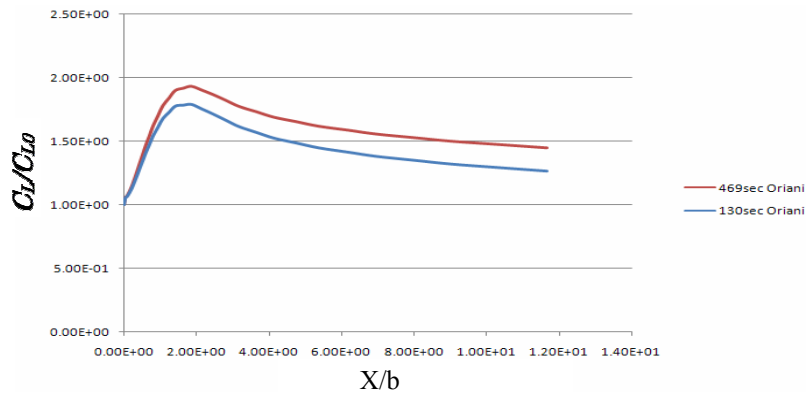


Fig. 7 Normalized lattice concentration (C_L/C_{L0}) ahead of the crack tip by our Oriani based scheme for a higher loading time.

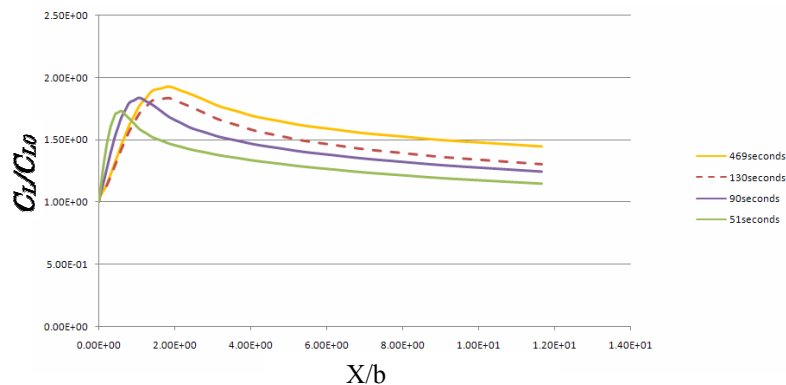


Fig. 8 Influence of the loading time on the hydrogen concentration distribution in lattice sites near the crack tip using the McNabb-Foster formulation ($k=2.8 \times 10^{-21} \text{ m}^3 \text{ s}^{-1}$).

If we compare the results of our one-way coupled analysis i.e. ignoring the effect of the diffusion field on the structural field using the McNabb-Foster formulation for hydrogen in lattice sites (see **Fig. 6**) with the results obtained by a fully coupled analysis i.e. considering the effect of diffusion field on the structural analysis based on the Oriani's theory, a similarity in the hydrogen

distribution for different loading times is observed in **Fig. 10** (see also **Fig. 6**). **Figure 10** is taken from Kanayama et al.'s paper ¹⁶⁾ for hydrogen concentration in lattice sites ahead of the crack tip after loading to $K_I = 40 \text{ MPa}\sqrt{\text{m}}$ which is much lower than K_I value in the current analysis. Therefore, the results should be compared qualitatively rather than quantitatively. The similar pattern of hydrogen distribution in **Figs. 6** and **10** is probably due to the fact that the quantity of hydrogen in our one-way coupled analysis using the McNabb-Foster formulation and in the fully-coupled analysis using the Oriani's equilibrium theory is more realistic than the one computed by a one-way coupled analysis based on the Oriani's theory.

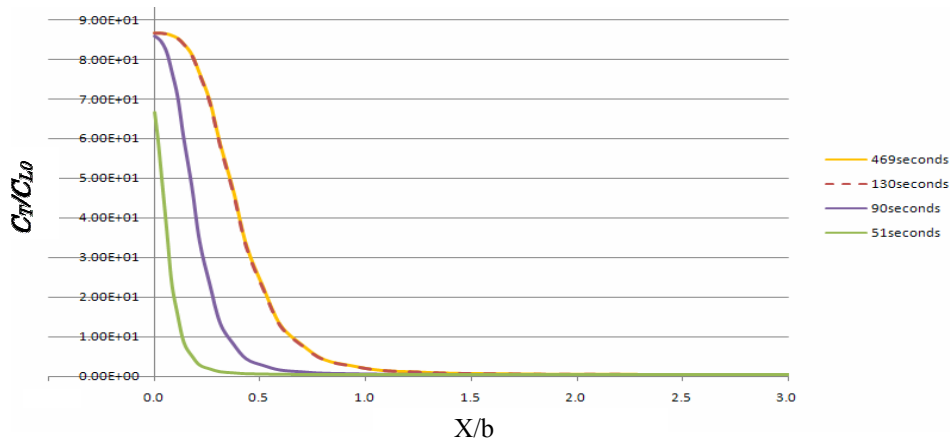


Fig. 9 Influence of the loading time on the hydrogen concentration distribution in trap sites near the crack tip using the McNabb-Foster formulation ($k=2.8 \times 10^{-21} \text{ m}^3 \text{ s}^{-1}$).

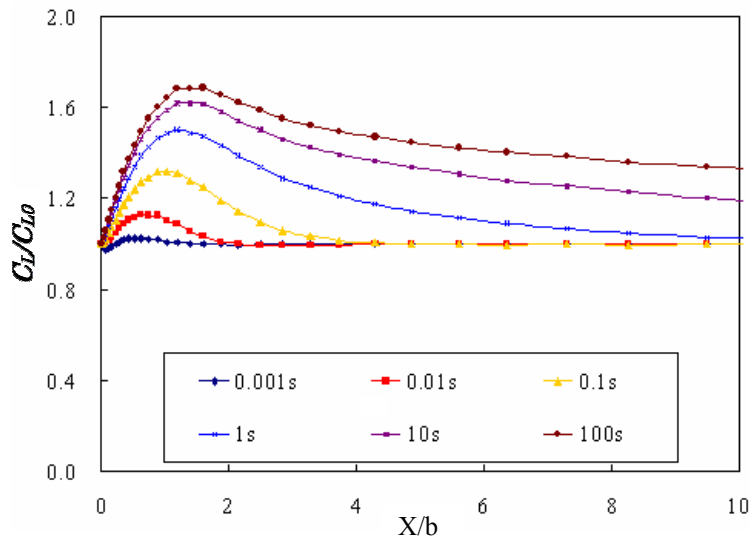


Fig. 10 Distribution of the normalized lattice hydrogen concentration for different loading times in a fully-coupled analysis based on the Oriani's equilibrium theory ^{16,17)}.

5. Conclusion

Following Sofronis ⁹⁾, we have reconsidered the transient advection diffusion equation by the McNabb-foster formulation to solve the boundary value problem of large strain

elastoplasticity-transient hydrogen diffusion analysis in the vicinity of a blunting crack tip under mode I (tensile) opening and small scale yielding conditions ¹⁴⁾, and compared the results with the one of using the Oriani equilibrium theory. The paper confirms the influence of the plastic strain rate term introduced by Krom et al. ⁷⁾ even in the reconsidered equation using the McNabb-Foster formulation. The results show a good agreement between the Oriani's equilibrium theory and the McNabb-Foster formulation in both trap and lattice site concentrations for sufficiently long loading times. In other words, for the sufficiently long loading times, the trapping of hydrogen can be assumed as a function of lattice concentration as it is the case in the Oriani's equilibrium theory. It is shown that the local equilibrium between hydrogen concentration in lattice sites and trap sites can only be assumed for the certain level of the plastic strain rate lower than 0.01 s^{-1} .

For the different loading times, the hydrogen distribution in lattice sites using the McNabb-Foster formulation in a one-way coupled analysis i.e. ignoring the effect of hydrogen on structural field is similar to the hydrogen distribution for a fully-coupled analysis based on the Oriani's theory ^{16,17)}. However, the hydrogen distribution in trap sites remains different since the basic principle in the Oriani's equilibrium theory is to consider the equilibrium between the lattice and the trap sites. The results obtained by the modified hydrogen diffusion model using the McNabb-Foster formulation confirm the hypothesis that for the small loading times i.e. high value of plastic strains, the Oriani's equilibrium theory is no longer dominant and the results should be verified by the McNabb-Foster formulation.

As a conclusion, on the one hand, the current study can be classified as a numerical development of the HELP theory, which implements the Sofronis and McMeeking's model ⁶⁾ to reconsider the advection diffusion equation by the generalized McNabb-Foster formulation in order to extend the theory of nonequilibrium trapping situations which is not included in the Oriani's theory. On the other hand, this paper may be nominated as an application for the McNabb-Foster formulation in the HELP theory. Moreover, the paper illustrates the criteria of the validity of the Oriani's equilibrium theory by considering the different loading times. In other words, it shows that the Oriani's theory seems to produce unreliable results when it comes to calculate the trap concentration in high rate of plastic strain. Current work represents an application of the McNabb-Foster formulation as a direct way to determine the trap site concentration in the HELP theory. Considering the nonequilibrium trapping situations, total hydrogen concentration which consists of both lattice and trap site concentrations has a significant effect on hydrogen embrittlement and must be determined precisely. According to this paper, using the McNabb-Foster formulation seems to be a good successor for the Oriani formulation particularly in small loading times (high rate of plastic strain) to determine a precise trap site concentration.

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References

- 1) Hirth, J.P., Effects of hydrogen on the properties of iron and steel, *Metallurgical and Materials Transactions A*, Vol. 11, Number 6, pp. 861-890 (1980).

- 2) Nagumo, M., Fundamentals of Hydrogen Embrittlement, Uchida Rokakuho Publishing Co. LTD., (2008 in Japanese).
- 3) Tabata T, Birnbaum H.K., Direct observations of the effect of hydrogen on the behavior of dislocations in iron, *Scripta Metall.*, Vol. 17, pp. 947-950 (1983).
- 4) Birnbaum, H.K., Sofronis, P., Hydrogen-enhanced localized plasticity—a mechanism for hydrogen-related fracture, *Materials Science and Engineering: A*, Vol. 176, pp. 191-202 (1994).
- 5) Sofronis, P., Birnbaum, H.K. Mechanics of the hydrogen-dislocation-impurity interactions-I. Increasing shear modulus, *Journal of the Mechanics and Physics of Solids*, Vol. 43, pp. 49-90 (1995).
- 6) Sofronis, P., McMeeking, R. M., Numerical analysis of hydrogen transport near a blunting crack tip, *Journal of the Mechanics and Physics*, Vol. 37, pp. 317-350 (1989).
- 7) Krom, A. H. M., Koers, R. W. J., Bakker, A., Hydrogen transport near a blunting crack, *Journal of the Mechanics and Physics of Solids*, Vol. 47, pp. 971-992 (1999).
- 8) Kanayama, H., Shingoh, T., Ndong-Mefane, S., Ogino, M., Shioya, R., Kawai, H., Numerical analysis of hydrogen diffusion problems using the finite element method, *Journal of Theoretical and Applied Mechanics*, Vol. 56, pp. 389-400 (2008).
- 9) Sofronis, P., Mechanics of hydrogen embrittlement, *Ph.D. Dissertation, University of Illinois at Urbana-Champaign*, Urbana, Illinois (1987).
- 10) Oriani, R. A., The diffusion and trapping of hydrogen in steel, *Journal of Acta Metallurgica*, Vol. 18, pp. 147-157 (1970).
- 11) McNabb, A., Foster, P. K., A new analysis of the diffusion of hydrogen in iron and ferritic steels, *Journal of Transaction of the Metallurgical Society of AIME*, Vol. 227, pp. 618-627 (1963).
- 12) Ndong-Mefane, S., Kanayama, H., Ogino, M., El-Amin, M. F., A stabilization method for the hydrogen diffusion model in materials, *Journal of Computational Science and Technology*, Vol. 2, No. 4, pp. 447-458 (2008).
- 13) Krom, A. H. R., Numerical modeling of hydrogen transport in steel, *Ph.D. Dissertation, Delft University of Technology*, Netherlands (1998).
- 14) Miresmaeili, R., Ogino, M., Shioya, R., Kawai, H., Kanayama, H., Finite element analysis of the stress and deformation fields around the blunting crack tip, *Memoirs of the Faculty of Engineering, Kyushu University*, Vol. 68, No. 4, pp. 151-161 (2008).
- 15) Sleijpen, G.L.G., Fokkema, D.R., BiCGSTAB(L) for linear equations involving unsymmetric matrices with complex spectrum, *Electronic Transactions on Numerical Analysis*, Vol. 1, pp. 11-32 (1993).
- 16) Kanayama, H., Ogino, M., Miresmaeili, R., Nakagawa, T., Toda, T., Hydrogen transport in a coupled elastoplastic-diffusion analysis near a blunting crack tip, *Journal of Computational Science and Technology*, Vol. 2, No. 4, pp. 499-510 (2008).
- 17) Kotake, H., Matsumoto, R., Taketomi, S., Miyazaki, N., Transient hydrogen diffusion analyses coupled with crack-tip plasticity under cyclic loading, *International Journal of Pressure Vessels and Piping*, Vol. 85, issue 8, pp. 540-549 (2008).