Modelling of Hydrogen Assisted Stress Corrosion Crack Extension along Centerline of Austenitic Stainless Steel Welds *Ishwar Londhe¹, † S. K. Maiti ²

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Abstract

This paper presents a numerical scheme for modelling hydrogen assisted stress corrosion cracking (HASCC) along centerline of gas tungsten arc (GTA) welds of austenitic stainless steel 21Cr-6Ni-9Mn (21-6-9). FEM based cohesive zone modelling (CZM) is used to examine the crack extension through the weld fusion zone (FZ). Diffusion of hydrogen through the lattice is analyzed by finite difference method incorporating effects of hydrostatic stress σ_h . J versus crack extension curves are obtained. Results are presented by considering both constant diffusivity and its variation with hydrogen concentration. The results based on the later case compare well with published experimental data. Analysis is also carried out to include effects of size and shape of FZ and heat affected zone (HAZ) on J- Δa variations. Temporal variations of hydrogen concentration and σ_h along the crack line ahead of the tip at various stages of crack extension are included.

Keywords: Hydrogen assisted stress corrosion cracking, cohesive zone modelling, J- Δa variation, FZ, HAZ, fracture initiation toughness.

1. Introduction

Austenitic stainless steels consists of 16-26% Cr, 8-24% Ni + Mn, up to 0.40% C and small amounts of a few other elements such as Mo, Ti, Nb and Ta. The steel contains about 90-100% of austenitic microstructure which is made possible by adjusting the amount of Cr and Ni + Mn. These alloys provide good strength and high toughness over a wide temperature range and oxidation resistance to little over 1000°F. Due to such excellent properties, they are mostly employed in machines, pipelines and structures subjected to hydrogen and other corrosive environments. During welding of such steels Cr content in base metal is generally kept high in filler wire as Cr is ferrite stabilizer whereas Ni is austenite stabilizer. After welding of austenitic steel and during solidification, melting of certain low melting point constituents like sulfur, phosphorous, manganese and silicon cause shrinkage induced strain. δ -ferrite has capacity to dissolve such harmful elements. Hence, residual amount of stable δ ferrite is always preferred in steel microstructure to prevent hot cracking [1]. But, it is also reported that δ -ferrites are the dominating sites for microcrack formation and its propagation under load [2]. Weld joints of the austenitic stainless steels therefore becomes weaker against HASCC due to retained δ -ferrite. A common source of hydrogen during welding is the flux used which has ingredients containing chemically bonded water (H₂O) in their microstructure. This water dissociates as hydrogen and oxygen at high temperatures. Ingress of hydrogen is facilitated further by increase of hydrogen solubility in steel with increasing temperature. If the cooling is slow, some of the dissolved hydrogen may escape to the atmosphere; if the cooling is fast then there is no such possibility [3].

Several experiments [2][4][5] have shown that the dominant sites for initiation of microcracks are the ferrite and ferrite-austenite boundaries in the weld microstructure. The microcracks gradually develop into macro-cracks, which grow subsequently both along, and perpendicular to, the initial crack line/plane. A 2-D analysis of such a crack growth only along the weld centerline, which is a FZ, is the objective of this study.

Analysis of the problem is difficult because of existence of three distinct material zones, i.e. FZ, HAZ and the base metal (BM). Fracture in such steels is a complex phenomenon involving ferrite, austenite-ferrite boundary, micro-crack formation, shear linkage between micro-cracks [2]. Both tensile and H₂ diffusion properties also differ from one zone to another. There is not much published data on the properties except some experimental results on variation of J with crack extension [2][4]. The study of the problem is further complicated by the fact that the corrosion affects the crack extension and the later, in turn, affects the diffusion and corrosion. The two phenomena are therefore coupled. The analysis of such a problem through homogenous material in the presence of HASCC has been reported earlier by several investigators. Both sequential [6][7] and coupled analysis have been reported [8]. A sequential analysis of a crack propagation along the weld centerline is considered in this paper. Due to non-availability of all required exhaustive material properties/data, e.g., tensile strength, % elongation, diffusivity parameters, reduction of cohesive strength with hydrogen concentration, etc., the appropriate data are iteratively adjusted to get the best predictions for J vs. Δa variations. In the modelling, variation of yield strength across the HAZ has been interpolated linearly from $\sigma_{\rm Y}$ = 485 MPa at the interface of HAZ and BM to $\sigma_{\rm Y}$ = 675 MPa at the interface of FZ and HAZ. The case studies presented here concerns internal hydrogen assisted corrosion (IHAC) in CT specimen with crack along the centerline of the weld. The complex failure mechanism is modelled using a hydrogen concentration dependent cohesive zone modelling technique (HCD-CZM).

2. Experimental Details

The experimental results of Somerday et al. [4] provide the basis for the present analysis. Similar studies were also carried by Jackson et al. [5] and Nibur et al. [9] for 304L/308L and 21Cr-6Ni-9Mn/308L austenitic stainless steel welds respectively. The base metal for the present analysis is 21Cr-6Ni-9Mn (21-6-9) steel, which was available in the form of rectangular bar stock of size 75×75 mm.



Figure 1. a) Macrograph of 21-6-9/21-6-9 GTA weld [4] and (b) CT specimen considered for modelling the weld

The details of preparation of specimen and testing is given in [4]. It suffices to state here that, in order to prepare the weld, a tapered "U" groove was made at the centre of a rectangular bar stock (Fig. 1a). This groove was filled with 21-6-9 filler wire by GTA welding operation. A standard CT specimen was then cut out of the bar stock. The machined specimen was provided with a 45° side groove. Based on the overall dimensions provided in [4], dimensions of a typical specimen are: width (W) = 26.5 mm, nominal thickness (B) = 6 mm, reduced thickness near the weld (B_c) = 4.6 mm and pre-crack length to specimen width ratio (a/W) = 0.50.

Before the actual testing pre-cracking was appropriately done ahead of the machined notch. Specimens were then kept in hydrogen bath for charging for 29 days to reach a uniform hydrogen concentration of 230 ppm (by weight) and tested at loading rates of 0.4 and 0.04 mm/min [4]. The J integral (J) vs crack extension (Δa) curves are reproduced in Fig. 2. These clearly shows that hydrogen reduces the fracture initiation toughness as well as the slope of crack growth resistance curve significantly. Fracture initiation toughness (J_Q) dropped by more than 53 % for the specified pre-charging in comparison with charge-free specimens (Fig. 2) [4].



Figure 2. J vs ∆a curves for 21-6-9/21-6-9 GTA weld [4]

3. Finite Element (FE) Model

3.1 CT specimen geometry and model

Only one half of the specimen is considered for analysis. Figs. 3, 4 and 5 shows the details of three geometries of FZ, HAZ and BM considered for the simulation. Fig. 3 considers a quadrilateral FZ where as Figs. 4 and 5 consider respectively a rectangular and triangular fusion zone. The dimensions of the three zones were approximated from the photograph of the specimen (Fig. 1a) using a plot digitizer software. The fusion and heat affected zones exhibit very different mechanical properties than that of the base metal. For example, the fusion zone exhibits a typical cast structure while heat affected zone exhibits a heat-treated structure involving phase transformation, recrystallization and grain growth. The BM and FZ have yields strength ($\sigma_{\rm Y}$) of 485 MPa and 675 MPa respectively [12]. Young's modulus (E) of the two materials is 196.6 GPa and the Poisson's ratio is 0.3 [4]. Over the HAZ, as



mentioned earlier, the material properties are assumed to vary linearly from $\sigma_{\rm Y}$ = 485 MPa at the interface of HAZ and BM to $\sigma_{\rm Y}$ = 675 MPa at the interface of FZ and HAZ.





(All dimensions are in mm)

3.2 TSL parameters (T_0 , δ_0)

In the present analysis the TSL employed is similar to the one used by Raykar et al. [13] and Scheider et al. [14]. This type of TSL introduces flexibility as the TSL shape can be varied easily by changing parameters δ_1 and δ_2 (Fig. 6). The two important TSL parameters, traction (T_0) and critical separation displacement $(\delta_0),$ were settled by analyzing the case of crack propagation through the quadrilateral FZ without any hydrogen charging and comparing the predicted J vs. Δa variations with the corresponding experimental data (Fig. 2). The analysis under IHAC condition was done by



replacing T_0 by T_0 (1- μ C). Actual traction separation variation for uncharged and charged cases are shown schematically in Fig. 6. The exact form of TSL is given below.

$$T = T_0 (1 - \mu C) \begin{cases} 2 \left(\frac{\delta}{\delta_0} \right) - \left(\frac{\delta}{\delta_0} \right)^2, & \delta < \delta_1 \\ 1, & \delta_1 < \delta \le \delta_2 \\ 2 \left(\frac{\delta - \delta_0}{\delta_0 - \delta_2} \right)^3 - 3 \left(\frac{\delta - \delta_0}{\delta_0 - \delta_2} \right)^2, & \delta_2 < \delta \le \delta_0 \end{cases}$$
(1)

As can be seen from this equation, the term μC affects the cohesive strength (T). The reduction factor μ in the cohesive strength is considered constant for a particular loading rate.

It is settled by comparing the predicted J vs. Δa variations with the corresponding experimental values for hydrogen charged specimens. $\mu=0$ corresponds to testing under charge-free conditions. The hydrogen concentration (C) in Eqn. (1) is not constant for a given loading rate; it varies with time at any node of a cohesive element.

3.3 Mesh size determination

The specimen was discretized in such a way that top layer (Fig. 7) consists of cohesive elements of zero thickness. These elements are placed along the crack propagation direction as shown. Just below these elements, there are few layers of refined continuum elements; rest of the specimen have comparatively coarser mesh. The mesh size near the crack tip was fine enough to capture the stress distribution accurately around the crack tip.

The side groove was accommodated by considering a 3-step variation of thickness (Fig. 3) of normal elements immediately below the cohesive element. The depth of the top two layers is 0.145 mm each and their widths are 4.6 mm and 5.3 mm respectively. The cohesive element width is therefore 4.6 mm. The size of continuum and cohesive elements along the crack propagation direction were arrived at by trial and error by comparison of predicted and experimental J vs. Δa diagrams for charge free specimens for loading rate of 0.4 mm/min (Fig. 7).



Figure 7. Mesh discretization of CT specimen

Case studies were performed by considering various combination of sizes for cohesive and continuum elements (Figs. 8, 9). Continuum elements are 4 noded quadrilateral plane stress

elements (CPS4 of ABAQUS[®] software). Cohesive elements are 2 noded linear elements (COH2D4 of ABAQUS[®] software). From Figs. 8 and 9, it is observed that the optimum size of continuum and cohesive elements are 0.1 mm and 0.02 mm respectively.



variable continuum element size

4. Analysis of hydrogen charged specimens

When a charged specimen is tested, hydrogen concentration keeps changing near the crack tip because there is mobility of hydrogen atoms towards the location of high stress concentration. The equation governing this movement was first given by Sofronis and McMeeking [15] in the form given below.

$$\frac{\partial C_L}{\partial t} = D_{eff} \frac{\partial^2 C_L}{\partial x^2} - D_{eff} \frac{V_H}{RT} \frac{\partial C_L}{\partial x} \frac{\partial \sigma_h}{\partial x} - D_{eff} \frac{V_H C_L}{RT} \frac{\partial^2 \sigma_h}{\partial x^2} = 0,$$
(2)

where x is the distance from the crack tip along the crack path, σ_h is hydrostatic stress. *R*,*T* and D_{eff} are the universal gas constant, absolute temperature, effective diffusivity of hydrogen respectively. V_H (= 2×10³ mm³/mol) is partial molar volume of hydrogen in the metal at temperature (*T*) of 300K. C_L and C_T are the number of hydrogen atoms per unit volume present in the lattice and trap sites respectively.

 $C_L = \theta_L \beta N_L$. β denotes number of normal interstitial lattice sites (NILS) per solvent atom, θ_L denotes the fraction of the NILS occupied by lattice hydrogen atom and N_L is the number of solvent lattice atoms per unit volume. Parameters β and N_L are constant for a given lattice; β is taken as 1. Similarly C_T can be expressed as $\theta_T \alpha N_T$. α signifies number of hydrogen atoms per trap, θ_T is trap occupancy and N_T is number of traps per unit lattice volume [4]. α is taken as 10. C_T is related to C_L by Oriani's law [16] as follows.

$$C_{T} = \frac{K_{tr} \left(\frac{\alpha . N_{T}}{\beta . N_{L}}\right) C_{L}}{1 + \left(\frac{K_{tr}}{\beta . N_{L}}\right) C_{L}},$$
(3)

where $K_{tr} = e^{\frac{E_B}{RT}}$. K_{tr} is trap equilibrium constant which depends upon the trap binding energy (E_B) for hydrogen atoms and absolute temperature (T). When E_B is small, the trap is called as irreversible trap; this type of trap sites releases hydrogen and causes more damage. $E_B = 60$ kJ is considered as the upper limit for binding energy for reversible trap sites [22]. E_B and T for 21-6-9 austenitic stainless steel are given as 9.65 kJ/mol and 298K respectively [3].

 N_T is dependent upon plastic strain (ε_p) . The relation between N_T and ε_p is given by McMeeking [15] and Krom et al. [17] as follows.

$$\log N_T = 23.26 - 2.33e^{-5.5\varepsilon_p},\tag{4}$$

$$N_L = \frac{N_A}{V_M},\tag{5}$$

where N_A is the Avogadro's number (6.023×10²³) and V_M is the molar volume of the host lattice (7.116×10⁻⁶ m³/mol). The effective diffusivity (D_{eff}) is given by Sofronis and McMeeking [15].

$$D_{eff} = D_L \frac{C_L}{C_L + C_T (1 - \theta_T)},$$
(6)

where D_L is the lattice diffusivity of hydrogen atoms and $\theta_T = \frac{C_{TO}}{\alpha N_T}$. In the present analysis total hydrogen concentration is normalized as follows.

$$C = \frac{C_L + C_T}{C_{LO} + C_{TO}},$$
(7)

where C_{L0} and C_{T0} are stress free equilibrium solubility of hydrogen in iron at 300K. Value of C_{L0} is taken as 2.0845×10^{21} atoms/m³ [15]. C_{T0} is obtained through Eqn. (3) as 2.203×10^{17} atoms/m³. Further, the initial hydrogen concentration has been taken to be equal to specified concentration C_{L0} throughout the domain.

Based on the observation that, for a two dimensional problem of a homogenous material, 1-D analysis of diffusion along the crack line is quite sufficient [13][14], 1-D form of diffusion Eqn. (2) was solved by finite difference method. In the present study results are obtained by considering the diffusivity to be constant in one case and variable in the other.

4.1 Solution of 1-D diffusion considering constant diffusivity (D_{eff})

One dimensional form of hydrogen diffusion equation with the inclusion of hydrostatic stress σ_h is obtained from Eqn. (2) as follows [13].

$$\frac{\partial C_L}{\partial t} = D_{eff} \frac{\partial^2 C_L}{\partial x^2} - E_H \frac{\partial C_L}{\partial x} \frac{\partial \sigma_x}{\partial x} - E_H C_L \frac{\partial^2 \sigma_h}{\partial x^2}, \tag{8}$$

where \mathcal{X} is measured from crack tip and $E_H = \frac{D_{eff}V_H}{RT}$.

This equation was solved numerically using Crank-Nicholson scheme (central difference method) along the line of Raykar et al. [13]. Let $(C_L)_j^n$ be the magnitude of C_L at time step n; j = 1, 2, 3... are the grid points; Δt is the time interval between (n+1)th and nth step. Δx is equal to width (0.02 mm) of cohesive elements. Total number of grid points considered is 131, i.e., maximum value of j=131. The lattice concentration of hydrogen at a given location $((C_L)_i^n)$ and at the two time steps n and n+1 are related.

$$\frac{(C_{L})_{j}^{n+1} - (C_{L})_{j}^{n}}{\Delta t} = D_{eff} \left\{ \frac{\left[(C_{L})_{j+1}^{n+1} - 2(C_{L})_{j}^{n+1} + (C_{L})_{j+1}^{n+1} \right] + \left[(C_{L})_{j-1}^{n} - 2(C_{L})_{j}^{n} + (C_{L})_{j+1}^{n} \right]}{2\Delta x^{2}} \right\} - E_{H} \left\{ \frac{\left[(C_{L})_{j+1}^{n+1} - (C_{L})_{j-1}^{n+1} \right] + \left[(C_{L})_{j+1}^{n} - (C_{L})_{j-1}^{n} \right]}{4\Delta x} \right\} \left\{ \frac{(\sigma_{h})_{j+1}^{n} - (\sigma_{h})_{j-1}^{n}}{2\Delta x} \right\} - E_{H} \left\{ \frac{\left((C_{L})_{j+1}^{n+1} + (C_{L})_{j}^{n} \right)}{2} \right\} \left\{ \frac{(\sigma_{h})_{j+1}^{n} - 2(\sigma_{h})_{j}^{n} + (\sigma_{h})_{j-1}^{n}}{(\Delta x)^{2}} \right\} \right\}$$
(9)

This relation is obtained through the Crank-Nicholson scheme. With the following substitutions,

$$\alpha_1 = \frac{D_{eff}\Delta t}{2\Delta x^2} \tag{10}$$

$$\beta_{1} = \frac{E_{H}\Delta t}{8\Delta x^{2}} ((\sigma_{h})_{j+1}^{n} - (\sigma_{h})_{j-1}^{n})$$
(11)

$$\gamma_{1} = \frac{E_{H}\Delta t}{2\Delta x^{2}} ((\sigma_{h})_{j=1}^{n} - 2(\sigma_{h})_{j}^{n} + (\sigma_{h})_{j+1}^{n})$$
(12)

the following simplified form is obtained from Eqn. (9).

$$(-\alpha_{1} - \beta_{1})(C_{L})_{j+1}^{n+1} + (1 + 2\alpha_{1} - \gamma_{1})(C_{L})_{j}^{n+1} + (-\alpha_{1} + \beta_{1})(C_{L})_{j-1}^{n+1}$$

$$= (\alpha_{1} + \beta_{1})(C_{L})_{j+1}^{n} + (1 - 2\alpha_{1} + \gamma_{1})(C_{L})_{j}^{n} + (\alpha_{1} - \beta_{1})(C_{L})_{j-1}^{n}$$
(13)

Eqn. (13) can be applied at a particular time step at all the grid points to get their hydrogen concentration at the time step (n+1). This process is repeated as many times as required in a case study. These hydrogen concentrations were utilized to amend the reduction in strength of material due to variations in hydrogen concentration and hydrostatic stress. This was adopted in the crack propagation analysis through ABAQUS[®] subroutine USDFLD.

4.2 Solution of 1-D diffusion equation considering variable diffusivity (D_{eff})

In this case the term D_{eff} is not constant but varies with change in level of C_L and C_T with time. This effect is introduced in the model by substituting D_{eff} in Eqn. (9) as follows.

$$D_{eff} = \frac{D_L \cdot (C_L)_j^{n+1}}{(C_L)_j^{n+1} + \frac{\frac{K_{tr} \alpha_{tr} N_T}{\beta N_L} \cdot (C_L)_j^{n+1}}{1 + \frac{K_{tr}}{\beta N_T} \cdot (C_L)_j^{n+1}} \cdot (1 - \theta_T)}$$
(14)

After substitution of Eqn. (14), Eqn. (9) gives rise to following non-linear relation in $(C_L)_j^{n+1}$. This was solved by Newton-Rhapson method following Kaiser et al. [18].

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$$\frac{(C_{L})_{j}^{n+1} - (C_{L})_{j}^{n}}{\Delta t} = \left\{ \frac{D_{L} (C_{L})_{j}^{n+1}}{\frac{K_{\nu} \alpha_{\nu} N_{T}}{(C_{L})_{j}^{n+1}} \cdot (C_{L})_{j}^{n+1}} \cdot (1 - \theta_{T})}{\left| \frac{K_{\nu} \alpha_{\nu} N_{T}}{(C_{L})_{j}^{n+1}} \cdot (C_{L})_{j}^{n+1}} \cdot (1 - \theta_{T}) \right|}{1 + \frac{K_{\nu}}{\beta N_{T}} \cdot (C_{L})_{j}^{n+1}} \cdot (1 - \theta_{T})} \right\}.$$

$$\left\{ \begin{cases} \left[\frac{(C_{L})_{j+1}^{n+1} - 2(C_{L})_{j}^{n+1} + (C_{L})_{j+1}^{n+1}} \right] + \left[(C_{L})_{j-1}^{n} - 2(C_{L})_{j}^{n} + (C_{L})_{j+1}^{n}} \right]}{2\Delta x^{2}} \right\} \\ - \frac{V_{H}}{RT} \left\{ \frac{\left[\frac{(C_{L})_{j+1}^{n+1} - (C_{L})_{j-1}^{n+1}} \right] + \left[(C_{L})_{j+1}^{n} - (C_{L})_{j-1}^{n}} \right]}{4\Delta x} \right\} \left\{ \frac{(\sigma_{h})_{j+1}^{n} - (\sigma_{h})_{j-1}^{n}}{2\Delta x} \right\} \\ - \frac{V_{H}}{RT} \left\{ \frac{(C_{L})_{j}^{n+1} + (C_{L})_{j}^{n}}{2} \right\} \left\{ \frac{(\sigma_{h})_{j+1}^{n} - 2(\sigma_{h})_{j}^{n} + (\sigma_{h})_{j-1}^{n}}}{(\Delta x)^{2}} \right\}$$

$$(15)$$

4.3 Boundary and initial conditions for diffusion analysis

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For the case of internal hydrogen assisted cracking (IHAC), it is assumed that the hydrogen is not allowed to diffuse out of the material (i.e. hydrogen flux is zero at crack tip and end of ligament). As the temperature of the specimen increases, the tendency of hydrogen to diffuse out of the specimen increases. To prevent hydrogen egress from the CT specimen, the temperature was maintained at 250 K after hydrogen pre-charging [4]. In the present model the boundary conditions employed are as follows. Both at the crack tip and ligament end, flux $(J_H) = 0$. That is,

$$D_L \nabla C_L - \frac{D_L C_L V_H}{RT} \nabla \sigma_h = 0, \qquad (16)$$

at both the locations.

For Eqn. (16) to be zero it is necessary that,

$$\left(\frac{\partial C_L}{\partial x}\right) = 0$$
, at the crack tip and the end of ligament (17)

$$\left(\frac{\partial \sigma_h}{\partial x}\right) = 0$$
, at the crack tip and the end of ligament (18)

These conditions are enforced by ensuring $C_L = C_{L0}$ at the first three (i.e., j = 1, 2, 3) and last three consecutive grid points (i.e., j = 129, 130, 131) (Fig. 10). The end conditions on hydrostatic stresses (Eqn. (18)) are similarly introduced. This small adjustment is implemented in ABAQUS[®] software through a user subroutine.

During the initial state, the specimen is fully charged with hydrogen, i.e., at t = 0, $C_L = C_{L0}$ throughout the crack plane. For incorporating the displacement boundary conditions, all the cohesive nodes are constrained in horizontal direction and can only exhibit separation in the vertical direction [19]. Displacement loading (at the rate 0.4 mm/min) is applied at the node representing the load point.



Exaggerated view of row of elements chosen for Hydrostatic stress extraction(at center of element)



Figure 10. Diagrammatic representation of boundary conditions

5. Comparison of simulation and experimental results

As per ASTM E1820 J is given as follows.

$$J = J_{elastic} + J_{plastic}, \tag{19}$$

where $J_{elastic}$ is represented by following equation.

$$J_{elastic} = (1 - \nu^2) \frac{K^2}{E},$$
 (20)

where E is Young's modulus and ν is the Poisson's ratio. K is the stress intensity factor which depends upon load (P) corresponding to a particular instant of crack extension (a), width of specimen (W), nominal thickness (B) and minimum thickness (B_c).

$$K = \frac{P}{\sqrt{BB_c W}} \frac{\left(2 + \frac{a}{W}\right)}{\left(1 - \frac{a}{W}\right)^{1.5} \left(0.886 + 4.64 \left(\frac{a}{W}\right) - 13.32 \left(\frac{a}{W}\right)^2 + 14.72 \left(\frac{a}{W}\right)^3 - 5.6 \left(\frac{a}{W}\right)^4\right)}$$
(21)

 $J_{plastic}$ is given by following equation.

$$J_{plastic} = \frac{n_p \times U_p}{B_c \times (W - a)},$$
(22)

where U_p is the total plastic energy calculated from load displacement plot, n_p is a factor given by Clarke and Landes [20]. It depends on specimen type and varies with crack size (a) and width of specimen (W) as follows.

$$n_p = 2 + 0.522 \left(1 - \frac{a}{W} \right) \tag{23}$$

5.1 Charge - free specimen

Initially a number of iterations were performed considering various shapes of FZ. The analysis was done considering the loading rate of 0.4 mm/min. Fig. 11 shows comparison of experimental and predicted J vs. Δa variations for three types of FZ shapes, i.e. rectangular, triangular and quadrilateral. The comparison is done for crack extension up to 1mm. The cohesive parameters are obtained comparing the predicted J vs. Δa variations with the corresponding experimental data for quadrilateral FZ are as follows: T₀ = 1241 MPa and $\delta_0/2$ = 0.0489 mm. These parameters are also used for rectangular and triangular FZs. The predictions based on the quadrilateral FZ (Fig. 3) compares most closely with the experimental results.

The fracture initiation toughness (J_Q) is defined by intersection of J resistance curve with 0.2 mm blunting line. For charge-free specimens and loading rate of 0.4 mm/min the experimental fracture initiation toughness is 439 kJ/m² [4]. The corresponding simulation results are 438.31 kJ/m², 739.08 kJ/m² and 787.65 kJ/m² for quadrilateral, rectangular and triangular FZs. This indicates errors of -0.16 %, +68.35 % and +79.42 % with respect to J_Q respectively. The maximum difference in the simulated result in the case of quadrilateral FZ is just +14.97 % at crack extension of 1 mm (Fig. 11). In the case of rectangular and triangular FZs, the maximum differences are +61.06 % and +59.37 % at crack extension of

0.3 mm. On the whole, the quadrilateral FZ gives better results. It is selected for the analysis of charged specimen too.



5.2 Charged specimen

The specimens with internal hydrogen assisted cracking (IHAC) were analyzed considering both constant diffusivity and variable diffusivity.

5.2.1 Constant Deff

As indicated earlier, during loading, hydrogen atoms move towards the crack tip, where there is high stress concentration. These movements were studied. Set of Eqns. (2-22) are considered in the analysis. The loading rate is 0.4 mm/min as before. Three D_{eff} values were considered. They were calculated from lattice diffusivity (D_L) using,

$$\begin{split} \mathcal{E}_{p} &= 0, \ N_{T} = 1.82 \times 10^{22}, \\ C_{T} &= C_{T0} = 2.2 \times 10^{17}, \\ C_{L} &= C_{L0} = 2.08 \times 10^{21}, \\ \theta_{T} &= \frac{C_{T0}}{\alpha N_{T}} = \frac{2.20 \times 10^{17}}{10 \times 1.82 \times 10^{22}} = 2.20 \times 10^{-6}, \\ D_{eff} &= D_{L} \frac{C_{L}}{C_{L} + C_{T} (1 - \theta_{T})} = D_{L} \frac{2.08 \times 10^{21}}{2.08 \times 10^{21} + 2.2 \times 10^{17} (1 - 1.2 \times 10^{-6})}, \\ &= 0.9999 \times D_{L} \approx D_{L}, \end{split}$$

This indicates that D_{eff} is almost the same as D_L . Analysis has been done for three trial values for D_L , 1.2×10^{-2} mm²/min, 1.2×10^{-3} mm²/min, 1.2×10^{-5} mm²/min [21].

 μ is varied in the range 0.2 to 0.6. The best value, based on comparison of predicted and experimental J vs. Δa is obtained as 0.28. The comparison of predicted and experimental J vs. Δa for three D_{eff} is presented in Fig. 12. This shows that $D_{eff} = 1.2 \times 10^{-3} \text{ mm}^2/\text{min}$ gives the best comparison with experimental data over the later stages of crack extension.



5.2.2 Variable Deff

In this case diffusivity is considered to be varying with the level of local hydrogen concentration. This method has the advantage that it eliminates the need for iterations to determine D_{eff} [18]. The iterations start with initial value of $D_{eff} = D_L$. Three D_L values are again considered, 1.2×10^{-2} mm²/min, 1.2×10^{-3} mm²/min, 1.2×10^{-5} mm²/min. The finite difference formulation of the resulting diffusion equation leads to a set of non-linear simultaneous equations. These equations are solved with appropriate initial and boundary conditions and are linked to the crack propagation analysis through ABAQUS[®] (version 6.11) user subroutine USDFLD. Table 1 gives the comparison of J values calculated by constant and variable diffusivity respectively.

By a suitable adjustment of the material data associated with diffusion and crack extension, better correlation is obtained for $D_L = 1.2 \times 10^{-5}$ mm²/min. A maximum difference of +19.85% in J is observed at $\Delta a = 0.16$ mm and the difference reduces to +1.46 % at the later stages (Table 1). The results further shows that, with the variable diffusivity, there is an overall improvement in comparison between experimental and predicted J vs. Δa variations for $D_L = 1.2 \times 10^{-5}$ mm²/min.

For charged specimens the experimental fracture initiation toughness is 100.75 kJ/m². The simulation yielded 109 kJ/m² for constant diffusivity ($D_{eff} = 1.2 \times 10^{-5} \text{ mm}^2/\text{min}$) and 108.94 kJ/m² for variable diffusivity ($D_L = 1.2 \times 10^{-3} \text{ mm}^2/\text{min}$). The crack extension (Δa) corresponding to fracture initiation toughness was taken as 0.26 mm [4].

Constant diffusivity ($D_{eff} = 1.2 \times 10^{-3} \text{ mm}^2/\text{min}$)				Variable diffusivity											
				$(D_L = 1.2 \times 10^{-5} \mathrm{mm^2/min})$				$(D_L = 1.2 \times 10^{-2} \mathrm{mm^2/min})$				$(D_L = 1.2 \times 10^{-3} \mathrm{mm^2/min})$			
Δa mm	Simulation J (kJ/m ²)	Experimental J (kJ/m ²)	%Error	∆a mm	Simulation J (kJ/m ²)	Experimental J (kJ/m ²)	%Error	∆a mm	Simulation J (kJ/m ²)	Experimental J (kJ/m ²)	%Error	∆a mm	Simulation J (kJ/m ²)	Experimental J (kJ/m ²)	%Error
0.16	106.30	88.66	19.89	0.16	106.26	88.66	19.85	0.16	106.20	88.66	19.78	0.16	106.29	88.66	19.88
S0. 28	109.54	103.21	6.14	0.30	110.01	103.21	6.59	0.22	107.33	95.83	12.00	0.3	110.09	103.21	6.67
0.48	115.65	113.69	1.73	0.48	115.35	113.69	1.46	0.30	108.71	103.21	5.33	0.38	112.46	109.50	0.35
0.68	123.22	127.27	-3.18	0.64	121.26	124.08	-2.27	0.40	110.69	110.46	0.21	0.54	117.82	117.06	0.66
0.80	129.65	136.34	-4.91	0.84	133.25	139.54	-4.51	0.62	115.97	130.45	-11.11	0.68	123.09	127.27	-3.29
0.90	138.05	144.35	-4.36	0.92	142.39	146.12	-2.55	0.78	121.03	134.34	-9.91	0.8	129.51	136.34	-5.01
0.94	147.67	147.90	-0.15	0.94	144.57	147.90	-2.25	0.90	125.65	144.35	-12.95	0.9	140.02	144.35	-3.00
1	162.39	153.23	5.98	1	161.09	153.23	5.13	1	131.88	153.23	-19.93	1	159.55	153.23	4.12

Table 1. Comparison of J at various stages of crack extension considering constant and variable diffusivity

The distribution of hydrogen concentration and hydrostatic stress (σ_h) ahead of the crack tip over a span along the crack line is presented (Fig. 13) at different stages of crack extension. The concentration of hydrogen (Fig. 13) reaches the highest value at a small distance from the instantaneous crack tip. This is very similar to a case reported earlier for hydrogen environment assisted cracking for a homogenous material [7]. The hydrostatic stress has the highest value close to the point of maximum C_L . This is because near the point of maximum hydrostatic stress, the lattice opens up the highest and has the maximum room for accommodation of hydrogen atoms. Thereby the hydrogen concentration becomes the maximum at this location [22].



Figure 13. Variation of hydrogen concentration and hydrostatic stress ahead of crack tip for constant D_{eff} (1.2×10⁻³ mm²/min)

5.3 Results for loading rate 0.04 mm/min

Similar analysis was also carried out for loading rate of 0.04 mm/min. The quadrilateral fusion zone was again considered and iterations were performed to fix cohesive strength reduction factor (μ). μ is obtained as 0.36. The simulation was carried out by considering variable diffusivity $D_L = 1.2 \times 10^{-5} \text{ mm}^2/\text{min}$. The analysis yielded fracture initiation toughness 78.92 kJ/m² compared with the experimental value 77.4 kJ/m².

6. Conclusions

In this study, an attempt has been made to examine the applicability of cohesive zone modelling to a heterogeneous specimen consisting of weld joint. The comparison (Table 1) indicates that a good prediction for J vs. Δa variation for the case of IHAC is possible with the help of CZM technique. The CZM parameters T₀ and δ_0 can be settled through combined numerical-experimental study. The same parameters can be employed for situations with

hydrogen charging. However, the cohesive strength reduction factor μ is required to be adjusted. This can be done through the combined numerical-experimental study.

For charged specimens, analysis has been carried out considering both constant and variable diffusivity. There is an overall reduction in error when the analysis is done considering the variable diffusivity. Further, there is better agreement between the experimental and predicted fracture initiation toughnesses for the two loading rates.

Out of the three shapes of weld fusion zones examined, i.e. triangular, rectangular and quadrilateral, the quadrilateral fusion zone gives the best comparison with experimental results.

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